

PSI-K

England & Wales · Charity number 1126308

Details

Status Registered

Legal form Charitable company

Company number [06440198](#)

Registered 2008-10-15

Register [View on the Charity Commission register](#)

Contact

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Keckwick Lane
Daresbury
Warrington
Cheshire
WA4 4AD

Phone 01925603602

Email psik-coor@dl.ac.uk

Website www.psi-k.org

Activities

Objects: FOR THE PUBLIC BENEFIT TO ADVANCE EDUCATION IN THE FIELD OF COMPUTATIONAL MATERIAL SCIENCE AND RELATED SUBJECTS, AND TO PROMOTE THE STUDY AND RESEARCH WORK IN THE FIELD OF MATERIAL SCIENCE AND RELATED SUBJECTS AND TO PUBLISH THE RESULTS OF EACH STUDY AND RESEARCH BY THE CO-ORDINATION OF AND COLLABORATION AND DISSEMINATION OF INFORMATION ON NAB INITIO COMPUTATIONAL MODELLING AMONG THE EUROPEAN RESEARCH COMMUNITY AND FROM THE RESEARCH COMMUNITY TO OTHERS OUTSIDE,THE MAINTENANCE AND ENHANCEMENT OF EUROPE'S STATUS AS THE LEADING RESEARCH AREA IN THE WORLD FOR COMPUTATIONAL MATERIALS SCIENCE FROM FIRST PRINCIPLES, THE PROMOTION OF RESEARCH,THE CONTINUOUS DEVELOPMENT OF THEORETICAL AND COMPUTATIONAL METHODOLOGY, THE PROMOTION AND CO-ORDINATION OF COLLABORATION WITHIN THE EUROPEAN RESEARCH COMMUNITY BY MEASURES INCLUDING,SUPPORTING, ORGANISING AND OTHERWISE BEING INVOLVED IN WORKSHOPS, CONFERENCES, SUMMER SCHOOLS, TUTORIAL COURSES, COLLABORATIVE EXCHANGE VISITS AND ANY OTHER TRAINING RELATED ACTIVITIES AND EVENTS,DISSEMINATING INFORMATION ABOUT SUCH ACTIVITIES AND EVENTS,DISSEMINATING OTHER RELEVANT INFORMATION INCLUDING BUT NOT LIMITED TO RESEARCH PROGRESS AND FUNDING OPPORTUNITIES,ENGAGING WITH THE WIDER SCIENTIFIC COMMUNITY, INDUSTRY, EUROPEAN POLICY MAKERS AND TRANS-EUROPEAN COMPUTER CENTRES, MAINTAINING CO-OPERATION WITH OTHER SCIENTIFIC AND RESEARCH ORGANISATIONS AND COMMUNITIES IN EUROPE AND THE WORLD,ADVANCING SUCH PURPOSES AS ARE CHARITABLE UNDER THE LAWS OF ENGLAND AND WALES.

Activities: Supports European research and researchers in materials through coordination of collaboration and dissemination of information on ab initio computational modelling among the European research community, and from the research community to others outside.

Classification

- **How:** Provides Services, Provides Advocacy/advice/information, Sponsors Or Undertakes Research, Acts As An Umbrella Or Resource Body
- **What:** Education/training
- **Who:** The General Public/mankind

Geography

- **Area of benefit:** UNDEFINED, IN PRACTICE
- Austria
- Belgium
- Czech Republic
- Denmark
- Finland
- France
- Germany
- Italy
- Luxembourg
- Norway
- Russia
- Spain
- Sweden
- Switzerland
- City Of London
- Warrington

Finances

Period end	Income	Expenditure	Assets	Employees
2024-12-31	£131,752	£98,553	-	-
2023-12-31	£122,216	£165,045	-	-
2022-12-31	£66,412	£98,137	-	-
2021-12-31	£155,651	£53,000	-	-
2020-12-31	£89,760	£132,471	-	-

Trustees

Name	Role	Appointed
Dr Arash Mostofi		2016-12-09
Dr James Kermode		2025-03-10
Dr Martin Friak		2024-11-29
Professor Claudia Draxl		2019-02-05
Professor Elisa Molinari		2019-02-14
Professor Emilio Artacho		2025-11-28
Professor Karsten Reuter		2024-11-29
Professor Lilia Boeri		2024-11-29
Professor Lucia Anna Reining		2019-02-14
Professor Mariana Rossi		2025-11-28
Professor Matthieu Verstraete		2025-11-28
Professor Patrick Rinke		2024-11-29
Professor Peter Haynes		2016-12-09
Professor Silke Biermann		2016-12-09
Professor Stefan Blugel		2017-11-24

PSI-K

England & Wales - Charity number 1126308

Accounts

Company registration number 06440198
Charity Commission number 1126308

PSI-K
(A company limited by guarantee)
REPORT AND UNAUDITED FINANCIAL STATEMENTS
YEAR ENDED 31 DECEMBER 2024

PSI-K
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YEAR ENDED 31 DECEMBER 2024

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**PSI-K
LEGAL AND ADMINISTRATIVE INFORMATION
YEAR ENDED 31 DECEMBER 2024**

Psi-k is a company limited by guarantee and a registered charity governed by its Memorandum and Articles of Association dated 29 November 2007.

Company registration number: 06440198

Charity registration number: 1126308

DIRECTORS AND TRUSTEES

The directors of the company are its Trustees for the purpose of Charity Law and throughout this report are collectively referred to as the Trustees. The Trustees who served during the period and to the date of this report are set on page 4.

SECRETARY

Damian Jones

REGISTERED AND PRINCIPAL OFFICE

Stfc Scitech Daresbury
Daresbury
Warrington
Cheshire
WA4 4AD

ACCOUNTANTS & INDEPENDENT EXAMINERS

RSM UK Tax and Accounting Limited
Chartered Accountants
Davidson House
Forbury Square
Reading
Berkshire
RG1 3EU

BANKERS

HSBC Bank Plc
11 Stamford New Road
Altrincham
Cheshire
WA14 1BW

**PSI-K
REPORT OF THE CHAIRMAN
YEAR ENDED 31 DECEMBER 2024**

During 2024, the Psi-k Charity supported a wide range of stimulating scientific and educational events. In total there were 22 workshops, summer schools and hands-on tutorials, the list of which can be found at <https://psi-k.net/psi-k-workshops-2024/>. The programme included the major annual research conference supported jointly with the European Centre for Atomic and Molecular Calculations (CECAM), on the topic of Electronic Structure Simulations for Large-Scale Facilities: Opportunities, Challenges and Roadmaps (<https://www.cecaml.org/workshop-details/electronic-structure-simulations-for-large-scale-facilities-opportunities-challenges-and-roadmaps-1207>); the 22nd International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods (<https://indico.ictp.it/event/10815>); and events specifically for training early-career researchers, including the 20th European Theoretical Spectroscopy Facility Young Researchers' Meeting (<https://lcpq.github.io/ym2024/>), and the Hands-on Workshop on Density Functional Theory and Beyond – from Foundations to Frontiers (<https://indico.ictp.it/event/a12198/>).

Three Psi-k Highlights were published during the course of the year: Understanding metal bonding, by Volker Heine and Siyu Chen; GPAW: an open python package for electronic structure calculations, by Jens Mortensen et al.; and Electronic structure calculations for muon spectroscopy, by Stephen Blundell et al., which can all be found at <https://psi-k.net/highlights/>, together with all Psi-k Highlights published from 1994 onwards. The Psi-k Highlight series showcases work that combines breadth and depth and is relevant to the Psi-k community. Suggested contributions can be discussed with leon.petit@stfc.ac.uk. We have established informal agreements with journals including npj Computational Materials and IOP Electronic Structure that provide opportunities for open-access publication of Psi-k Highlights

Psi-k's rich programme of activities is only made possible by generous membership donations from individuals and groups worldwide. In 2024, 35 groups or institutions from 14 countries contributed to the charity. Anyone (individuals, groups, organisations, companies) who would like to contribute may contact a.mostofi@imperial.ac.uk and PSIK_ADMIN@stfc.ac.uk, or contribute directly using PayPal via the link at <https://psi-k.net>.

The 22 Working Groups of Psi-k (<https://psi-k.net/groups/>) are organised by four main themes, each overseen by at least one Trustee (named in parenthesis):

- A. Physical formalisms – Lucia Reining and Silke Biermann
- B. Algorithms, software and data – Arash Mostofi and Stefan Blügel
- C. Applications to real materials and materials design – Martin Friak and Elisa Molinari
- D. Wider engagement – Peter Haynes

The Working Groups are instrumental in soliciting proposals for activities from the community, and assisting Trustees in evaluating proposals submitted in a two-step process: there is a first deadline at the end of July for outline proposals; these are evaluated and either encouraged to submit a full proposal by the end of October, rejected right away, or advised to merge with other efforts on similar themes to avoid duplication. The Psi-k/CECAM Research Conference has a separate track, and proposals not selected but deemed of sufficient quality can directly apply as a full proposal. This year Working Groups have also been closely involved in determining and developing the scientific programme for the next Psi-k Conference (which took place 25-28 August 2025 in Lausanne, Switzerland): Working Group leaders and representatives participated in the Programme Committee meeting in Lausanne in September that followed the worldwide call for topics and symposia.

A key milestone in 2024 was setting up a new mailing list for the Psi-k community. The old mailing list had grown beyond the capacity of the platform around which it was built and was no longer fit for purpose. Posts to the old mailing list were, therefore, suspended and a new mailing list was set up on Jiscmail, the UK's national academic mailing list service. I would like to thank members of the Psi-k Working Groups and Scientific Advisory Committee for beta-testing the new system before its wider release to the community. I would also like to thank Mike Towler for all his work and dedication in setting up and maintaining the old mailing list over many years.

PSI-K
REPORT OF THE CHAIRMAN (Continued)
YEAR ENDED 31 DECEMBER 2024

The Board of Trustees met five times in 2024, all by teleconference: on 9 February, 19 April, 21 June, 13 September and 8 November. Minutes of meetings are recorded, circulated, and kept for internal use. The Trustees (<https://psi-k.net/admin/>), plus Working Group leaders (<https://psi-k.net/groups/>) and members of the Scientific Advisory Committee (<https://psi-k.net/scientific-advisory-committee/>) attended the Annual Meeting on 22 November, where all activities are finalised for the following year (in this case, from April 2025 to March 2026).

The generous contribution of time from all the groups above is essential to the wellbeing of the charity, but particular thanks go to our long-serving Operations Manager Damian Jones (STFC Daresbury Laboratory, UK) who stepped down from the role this year. Thanks also go to Angelos Michaelides (Cambridge University, UK) who stepped down as a Trustee in June, the same month in which three new Trustees were appointed: Lilia Boeri (Sapienza University of Rome, Italy), Karsten Reuter (Fritz Haber Institute, Berlin, Germany), and Patrick Rinke (Technical University of Munich, Germany, and Aalto University, Finland).



Arash Mostofi - Psi-K Chair

25/09/25
Date:

**PSI-K
REPORT OF THE TRUSTEES
YEAR ENDED 31 DECEMBER 2024**

The Trustees present their annual report and unaudited financial Statements for the year ended 31 December 2024.

Trustees

The Trustees who served during the period and to the date of this report were:

Silke Biermann
Stefan Blügel
Lilia Boeri**
Claudia Draxl
Martin Friak
Peter Haynes
James Kermode***
Angelos Michaelides*
Elisa Molinari
Arash Mostofi (Chair)
Lucia Reining
Karsten Reuter**
Patrick Rinke**

*Angelos Michaelides resigned on 6th June 2024.

**Lilia Boeri, Karsten Reuter and Patrick Rinke were appointed as trustees on 21st June 2024.

*** James Kermode was appointed as a trustee on 10th March 2025.

Structure, governance and management

The organisation is governed by its Memorandum and Articles of Association and is a registered company limited by guarantee.

Psi-k is a Europe-based, worldwide network of researchers working on the advancement of first-principles computational materials science. Its mission is to develop fundamental theory, algorithms, and computer codes in order to understand, predict, and design materials properties and functions. Theoretical condensed matter physics, quantum chemistry, thermodynamics, and statistical mechanics form its scientific core. Applications encompass inorganic, organic and bio-materials, and cover a whole range of diverse scientific, engineering, and industrial endeavours. Key activities of Psi-k are the organisation of conferences, workshops, tutorials and training schools as well as the dissemination of scientific thinking in society.

Psi-k has a minimum of three Trustees, but there is no maximum. On the date of this report there were 12 Trustees.

Psi-k has a Chair, and a Scientific Advisory Committee (SAC) of about 80 members, which is headed by the Chair of Psi-k. All Trustees are also SAC members.

The Board of Trustees meets on average five to six times a year, normally with a combination of face-to-face meetings and teleconference meetings. In 2024 there were five meetings, all by teleconference: on 9 February, 19 April, 21 June, 13 September and 8 November. The Trustees had the opportunity to meet in person at the Annual Meeting of the SAC on 22 November. Minutes of meetings are recorded, circulated, and kept for internal use. The Board of Trustees uses these meetings to discuss matters including but not limited to: future strategy, funding and finances, events such as workshops, conferences and summer schools, and relationships with external organisations such as CECAM.

The day to day running of Psi-k is delegated to the Chair, Arash Mostofi. The Chair is supported by the Operations Manager. Damian Jones stepped down from this role in 2024, after over 15 years of service. Pankaj Pathania is the new Operations Manager and we welcome him warmly to the role.

The SAC meets once a year, normally in November, together with the leaders of the 22 Working Groups (<https://psi-k.net/groups/>). It is chaired by the Chair of Psi-k and its role is to make recommendations to the Board of Trustees, particularly regarding plans for all activities for the following year (in this case, from April 2025 to March 2026). In 2024 the Annual Meeting was held on 22 November in hybrid mode: in person in Paris and online.

These unaudited financial statements have been subjected to independent examination. See report on page 8.

PSI-K
REPORT OF THE TRUSTEES (Continued)
YEAR ENDED 31 DECEMBER 2024

All Trustees gave their time freely and no Trustee remuneration was paid in the year: expenses paid to Trustees amounted to €nil. Trustees are required to disclose all relevant interests and register them with the Chair.

Trustees are required to declare any conflicts of interest at each meeting and these are recorded in the minutes. If a vote of the Trustees is required on a matter, a Trustee who has declared a conflict of interest on that matter may not cast a vote.

Risk management

The Trustees have considered the major risks to which the charity is exposed and have reviewed those risks and established systems and procedures to manage those risks.

The Trustees have carefully considered the financial risks associated with the quinquennial Conference (to be next held 25-28 August 2025 in Lausanne) and consider them to be acceptable in view of the community benefit arising from a large, in-person conference, particularly for early career researchers and PhD students.

A significant risk for the Psi-k Charity is reduced financial funding. Since 2016, Psi-k has been sustained entirely by membership donations. In 2021 the Trustees agreed that our annual expenditure on community activities is determined by our income from the previous year, and adopted a target for reserves of €200,000.

Objectives and activities

Europe has become the leading research area in the world for the application of first-principles computational modelling to materials science and Psi-k aims to maintain and enhance this status.

“Psi-k research” covers structures, properties and processes in all types of materials at the atomic level and in nanometre-scale structures, studied by *ab initio* quantum-mechanical computer simulation. A series of working groups represent the views of the community and organise activities to deliver the Psi-k mission. These are:

Theme A: Physical Formalisms: Ground State and Spectroscopy of Many-Electron Systems	
WG A1	Density and density-matrix functional theories
WG A2	Perturbative many-body methods
WG A3	Non-perturbative many-body methods
WG A4	Open and non-equilibrium systems
WG A5	Phonons, electron-phonon coupling and related phenomena
Theme B: Algorithms, Software and Data	
WG B1	Multiscale and reduced-scaling methods
WG B2	Statistics and configuration sampling
WG B3	Software engineering
WG B4	High-throughput workflows and data analytics
WG B5	Artificial intelligence methods for materials genomics
Theme C: Applications to Real Materials and Materials Design	
WG C1	Structural materials
WG C2	Materials and devices for energy
WG C3	Quantum materials driven by correlations, topology or spin
WG C4	Catalysis and electrochemistry
WG C5	Materials for information and communication
WG C6	Nanoscale structures (2D, 1D, 0D) and related phenomena
WG C7	Molecules, macromolecules and biomolecules
Theme D: Wider Engagement	
WG B1	Social responsibility
WG B2	Early career researchers
WG B3	Industry engagement
WG B4	Training and education
WG B5	Policy engagement

These unaudited financial statements have been subjected to independent examination. See report on page 8.

PSI-K
REPORT OF THE TRUSTEES (Continued)
YEAR ENDED 31 DECEMBER 2024

Psi- k will promote and coordinate collaboration within the European research community by, among others, the following measures:

- supporting workshops and small conferences on specific topics of active research;
- supporting summer schools, tutorial courses and other training activities for early career and new researchers in the field;
- organising a large “Psi-k conference” every few years (such as those previously held in 1996, 2000, 2005, 2010, 2015 and 2022): the most recent was held in August 2025.
- disseminating information about research progress, job opportunities, relevant workshops, conferences and other events, and funding opportunities via the Psi-k website, providing a portal and a newsletter available freely to anyone in the world by electronic means.

The activities are open to all researchers in the field. Psi-k acts as a vehicle to engaging with the wider scientific community, with industry, European policy makers and trans-European computer centres. It will seek to maintain cooperation with organisations such as the Centre Européen de Calcul Atomique et Moléculaire (CECAM), the European molecular simulation community and its networks and Psi-k’s counterpart research communities on other continents.

Aims and objectives for 2024

The main activities planned during 2024 comprised the scientific programme of workshops, tutorials and summer schools on the electronic structure of complex processes in materials, i.e. the topic of the Psi-k Charity. The programme comprised 22 events, including the major annual research conference supported jointly with CECAM, the European Centre for Atomic and Molecular Calculations (CECAM), on the topic of Electronic Structure Simulations for Large-Scale Facilities: Opportunities, Challenges and Roadmaps (<https://www.cccam.org/workshop-details/electronic-structure-simulations-for-large-scale-facilities-opportunities-challenges-and-roadmaps-1207>).

Another key objective in 2024 was setting up a new mailing list for the Psi-k community to replace the old mailing list, which had grown beyond the capacity of the platform around which it was built and was no longer fit for purpose. The new mailing list was established in July on Jiscmail, the UK’s national academic mailing list service. The Trustees are grateful to members of the Psi-k Working Groups and Scientific Advisory Committee for beta-testing the new system before its wider release to the community. We would also like to thank Mike Towler for all his work and dedication in setting up and maintaining the previous mailing list over many years.

Grant making policy

The Psi-k Charity does not make grants to other research bodies.

The Psi-k Charity applies its funding to the organization of workshops, summer schools, hands-on courses and the Psi-k Conference. The Theoretical and Computational Physics Group at STFC Daresbury Laboratory publishes the Psi-k Newsletter and provides administrative support.

The achievements of every workshop to which Psi-k contributes are monitored in the form of a report which is published on the Psi-k website (<http://psi-k.net/>).

Key performance indicators

In 2024 the Psi-k Charity organised 22 workshops, conferences and training activities, which is in the middle of the typical range of 20 to 25 events and activities that have been supported in previous years.

Financial review 2024 and plan for 2025

Unrestricted net expenditure for the year was €22,509 (2023: €42,829). Unrestricted retained funds at the year end were €349,593 (2023: €372,102).

Membership donations in 2024 amounted to a total of €120,000 received (2023: €100,000). The expenses in the 2024 budget included €121,000 (2023: €120,000) for workshops.

Plan for 2025: The Trustees continue to seek new contributors with an aim of increasing annual membership donations to around €150,000. The amount of €122,000 will be spent for workshops in 2025. Any deficit will be covered by the reserves.

During the year 2024 the Trustees were satisfied that, as far as circumstances permitted, the Charity continued to benefit the public through its activities targeted to achieve its charitable objectives.

These unaudited financial statements have been subjected to independent examination. See report on page 8.

PSI-K
REPORT OF THE TRUSTEES (Continued)
YEAR ENDED 31 DECEMBER 2024

Public Benefit

The Trustees confirm that they have referred to the guidance contained in the Charity Commission's general guidance on public benefit when reviewing the Trust's aims and objectives and in planning future activities and setting the grant making policy for the year.

Trustees' responsibilities

The Trustees (who are also Directors of Psi-k for the purposes of company law) are responsible for preparing the Trustees' Annual Report and the financial statements in accordance with applicable law and United Kingdom Accounting Standards (United Kingdom Generally Accepted Accounting Practice).

Company Law requires the Trustees to prepare financial statements for each financial year which give a true and fair view of the state of affairs of the charitable company and of the incoming resources and applications of resources, including the income and expenditure, of the charitable company for that year. In preparing those financial statements, the Trustees are required to:

- provide statements on the going concern basis unless it is inappropriate to presume that the charitable company will continue in business;
- select suitable accounting policies and apply them consistently;
- observe the methods and principles in the Charitable SORP;
- make judgements and estimates that are reasonable and prudent;
- state whether applicable accounting standards have been followed, subject to any material departures disclosed and explained in the financial statements.

The Trustees are responsible for keeping proper accounting records that disclose with reasonable accuracy at any time the financial position of the charitable company and enable them to ensure that the financial statements comply with the Companies Act 2006. They are also responsible for safeguarding the assets of the charitable company and hence for taking reasonable steps for the prevention of fraud and other irregularities.

This report has been prepared in accordance with the Statement of Recommended Practice: Accounting and Reporting by Charities (issued in October 2019) and in accordance with the special provisions applicable to small companies.

ON BEHALF OF THE BOARD



Arash Mostofi (Chair)

Date: 25/09/25

INDEPENDENT EXAMINER'S REPORT TO THE TRUSTEES OF PSI-K

I report to the trustees on my examination of the financial statements of PSI-K ("the company") for the year ended 31 December 2024, which are set out on pages 9 to 16.

Responsibilities and basis of report

As the trustees of the company (and also its directors for the purposes of company law) you are responsible for the preparation of the financial statements in accordance with the requirements of the Companies Act 2006 ('the 2006 Act').

Having satisfied myself that the financial statements of the company are not required to be audited under Part 16 of the 2006 Act and are eligible for independent examination I report in respect of my examination of your charity's financial statements as carried out under section 145 of the Charities Act 2011 ('the 2011 Act'). In carrying out my examination I have followed the Directions given by the Charity Commission under section 145 (5)(b) of the 2011 Act.

An independent examination does not involve gathering all the evidence that would be required in an audit and consequently does not cover all the matters that an auditor considers in giving their opinion on the financial statements. The planning and conduct of an audit goes beyond the limited assurance that an independent examination can provide. Consequently, I express no opinion as to whether the financial statements present a 'true and fair view' and my report is limited to those specific matters set out in the independent examiner's statement.

Independent examiner's statement

I have completed my examination. I confirm that no material matters have come to my attention in connection with the examination giving me reasonable cause to believe that in any material respect:

1. accounting records were not kept in respect of the company as required by section 386 of the 2006 Act; or
2. the financial statements do not accord with those records; or
3. the financial statements do not comply with the accounting requirements of section 396 of the 2006 Act other than any requirement that the financial statements give a 'true and fair view' which is not a matter considered as part of an independent examination; or
4. the financial statements have not been prepared in accordance with the methods and principles of the Statement of Recommended Practice: Accounting and Reporting by Charities applicable to charities preparing their financial statements in accordance with the Financial Reporting Standard applicable in the UK and Ireland (FRS 102).

I have no concerns and have come across no other matters in connection with the examination to which attention should be drawn in this report in order to enable a proper understanding of the financial statements to be reached.

Kerry Gallagher

Name: **Kerry Gallagher FCA DchA**

Name of applicable listed body: **The Institute of Chartered Accountants in England and Wales**

Relevant professional qualification or membership of professional body: **Chartered Accountant**

ON BEHALF OF RSM UK TAX AND ACCOUNTING LIMITED

Chartered Accountants
Davidson House
Forbury Square
Reading
Berkshire
RG1 3EU
Date: 25/09/25

PSI-K
STATEMENT OF FINANCIAL ACTIVITIES
INCLUDING INCOME AND EXPENDITURE ACCOUNT
YEAR ENDED 31 DECEMBER 2024

	Notes	Unrestricted Funds €	Total Funds 2024 €	Total Funds 2023 €
INCOME				
Donations and legacies				
- Donated services		37,364	37,364	37,364
Charitable activities				
- Membership donations from research bodies		112,135	112,135	84,852
TOTAL INCOME		<u>149,499</u>	<u>149,499</u>	<u>122,216</u>
EXPENDITURE				
Charitable activities	4	172,008	172,008	165,045
TOTAL EXPENDEDITURE		<u>172,008</u>	<u>172,008</u>	<u>165,045</u>
NET INCOME/(EXPENDITURE) AND NET MOVEMENT IN FUNDS FOR THE YEAR		<u>(22,509)</u>	<u>(22,509)</u>	<u>(42,829)</u>
RECONCILIATION OF FUNDS				
TOTAL FUNDS BROUGHT FORWARD		<u>372,102</u>	<u>372,102</u>	<u>414,931</u>
TOTAL FUNDS CARRIED FORWARD	12	<u><u>349,593</u></u>	<u><u>349,593</u></u>	<u><u>372,102</u></u>

These unaudited financial statements have been subjected to independent examination. See report on page 8.

	Notes	2024 €	2023 €
CURRENT ASSETS			
Debtors	9	21,629	30,901
Cash at bank		563,196	522,906
		<u>584,825</u>	<u>553,807</u>
CURRENT LIABILITIES			
CREDITORS: Amounts falling due within one year	10	(235,232)	(181,705)
		<u></u>	<u></u>
NET CURRENT ASSETS		<u>349,593</u>	<u>372,102</u>
INCOME FUNDS			
Unrestricted funds	12	349,593	372,102
Restricted funds	12	-	-
		<u></u>	<u></u>
	12	<u>349,593</u>	<u>372,102</u>

For the year ending 31 December 2024 the company was entitled to exemption from audit under Section 477 of the Companies Act 2006 relating to small companies.

The members have not required the company to obtain an audit of its financial statements for the year ended 31 December 2024 in accordance with Section 476 of the Companies Act 2006.

The directors acknowledge their responsibilities for:

- ensuring that the company keeps accounting records which comply with Section 396 of the Companies Act 2006; and
- preparing financial statements which give a true and fair view of the state of affairs of the company as at the end of each financial year and of its profit or loss for each financial year in accordance with the requirements of Section 396 and which otherwise comply with the requirements of the Companies Act 2006 relating to financial statements, so far as applicable to the company.

These financial statements are prepared in accordance with the provisions applicable to companies subject to the small companies regime and in accordance with Charities SORP (FRS102).

The notes on pages 11 to 16 form part of these financial statements.

The financial statements were approved by the Trustees and authorised for issue on 25/09/25 and were signed on their behalf by:



Arash Mostofi (Chair)

Trustee

These unaudited financial statements have been subjected to independent examination. See report on page 8.

PSI-K
NOTES TO THE FINANCIAL STATEMENTS
YEAR ENDED 31 DECEMBER 2024

1. ACCOUNTING POLICIES

a. Basis of preparation

The financial statements have been prepared in accordance with Accounting and Reporting by Charities: Statement of Recommended Practice applicable to charities preparing their financial statements in accordance with the Financial Reporting Standard applicable in the UK and Republic of Ireland (FRS 102) (Issued October 2019) - (Charities SORP (FRS 102)), the Financial Reporting Standard applicable in the UK and Republic of Ireland (FRS 102) and the Companies Act 2006.

The financial statements are prepared in Euro and amounts in these financial statements are rounded to the nearest Euro.

PSI-K meets the definition of a public benefit entity under FRS 102. Assets and liabilities are initially recognised at historical cost or transaction value unless otherwise stated in the relevant accounting policy notes.

b. Preparation of the financial statements on a going concern basis

The trustees forecast that the charity will continue to be able to pay its liabilities as they fall due for a period of at least 12 months following the date of approving the financial statements. The forecasts take into account transactions that are anticipated to take place in the foreseeable future and indicate that no additional financial resources will be required should the actual performance differ from forecast. On this basis the trustees have concluded that adopting the going concern basis of accounting in preparing the annual financial statements is appropriate.

c. Income recognition

Incoming resources represents membership contributions from research bodies in Europe to support the company's activities, less amounts carried forward to future periods as deferred income; and donated services, which are included based on the hours worked and the appropriate hourly rate. Income is recognised when the entity has entitlement to the funds, it is probable that the income will be received and the amount can be measured reliably.

d. Donated services

Donated services are included within incoming resources with an equivalent amount shown within resources expended, where the benefit to the charity is reasonably quantifiable, measurable and material. The value placed on these resources is the estimated value to the charity of the service received.

e. Deferred income

Income received in advance of the period that it relates to, or is provided specifically for future periods, are carried forward as deferred income. These amounts relate to contributions from research bodies received in advance.

f. Expenditure recognition

All expenditure is accounted for on an accruals basis, inclusive of any VAT which cannot be recovered.

Grants payable are payments made to third parties in the furtherance of the charitable objectives of the Charity. Grants are accounted for when either the recipient has a reasonable expectation that they will receive a grant and the trustees have agreed to pay the grant without condition, or the recipient has a reasonable expectation that they will receive a grant and any condition attaching to the grant is outside of the control of the Charity.

Provisions for grants are made when the intention to make a grant has been communicated to the recipient but there is uncertainty about either the timing of the grant or the amount of grant payable.

Governance costs are related to the governance of the charity, such as the costs of preparing the financial statements and statutory compliance.

Irrecoverable VAT is charged as a cost against the activity for which the expenditure was incurred.

PSI-K
NOTES TO THE FINANCIAL STATEMENTS
YEAR ENDED 31 DECEMBER 2024

1. ACCOUNTING POLICIES (Continued)

g. Charitable Funds

Restricted funds are to be used for specified purposes as laid down by the donor. Expenditure which meets these criteria is identified to the fund, together with a fair allocation of management and support costs.

Unrestricted funds are available for use at the discretion of the Trustees in furtherance of the general objectives of the Charity.

h. Foreign currencies

The trustees consider that the functional currency of the charity is the Euro, as most transactions are denominated and are carried out in that currency.

Assets and liabilities denominated in other currencies are translated into Euros at the rate of exchange ruling at the balance sheet date. Transactions in other currencies are translated into Euros at the rate of exchange ruling at the date of the transaction. Exchange differences are taken into account in arriving at the net movement in funds in the Statement of Financial Activities.

At the balance sheet date the rate of exchange between Sterling and Euro was £1 equals €1.2097 (2023: €1.1505).

i. Financial instruments

The Charity has elected to apply the provisions of Section 11 'Basic Financial Instruments' and Section 12 'Other Financial Instruments Issues' of FRS 102, in full, to all of its financial instruments.

Financial assets and financial liabilities are recognised when the Charity becomes a party to the contractual provisions of the instrument, and are offset only when the Charity currently has a legally enforceable right to set off the recognised amounts and intends either to settle on a net basis, or to realise the asset and settle the liability simultaneously.

j. Basic Financial assets

Trade and other debtors (including accrued income) which are receivable within one year and which do not constitute a financing transaction are initially measured at the transaction price and subsequently measured at amortised cost, being the transaction price less any amounts settled and any impairment losses.

k. Basic Financial liabilities

Financial instruments are classified as liabilities according to the substance of the contractual arrangements entered into.

Trade and other creditors (including accruals) payable within one year that do not constitute a financing transaction are initially measured at the transaction price and subsequently measured at amortised cost, being the transaction price less any amounts settled.

l. Derecognition of financial liabilities

Financial liabilities are derecognised when the charity's contractual obligations expire or are discharged or cancelled

2. CRITICAL ACCOUNTING ESTIMATES AND JUDGMENT

In the application of the Charity's accounting policies, the trustees are required to make judgements, estimates and assumptions about the carrying amount of assets and liabilities that are not readily apparent from other sources. The estimates and associated assumptions are based on historical experience and other factors that are considered to be relevant. Actual results may differ from these estimates.

The estimates and underlying assumptions are reviewed on an on-going basis. Revisions to accounting estimates are recognised in the period in which the estimate is revised where the revision affects only that period, or in the period of the revision and future periods where the revision affects both current and future periods.

No critical accounting estimates and judgements have been made in preparing these financial statements.

PSI-K
NOTES TO THE FINANCIAL STATEMENTS
YEAR ENDED 31 DECEMBER 2024

3. INCOME

Membership donations received from research bodies attributable to overseas markets total 98% (2023: 96%). All income received in 2024 (and 2023) was unrestricted.

4. TOTAL EXPENDITURE

	Grant Funding of Activities €	Support Costs €	Total 2024 €	Total 2023 €
Charitable Activities				
Grants payable	121,700	-	121,700	111,450
Support costs	-	38,826	38,826	42,633
Exchange (gains)/losses	-	(140)	(140)	18
Governance Costs (Note 5)	-	11,622	11,622	10,944
	121,700	50,308	172,008	165,045

Total expenditure for the year was €172,008, all of which was unrestricted expenditure (2023: €165,045).

The grant funding of activities totalling €121,700 (2023: €111,450) relates to payments made to institutions regarding scientific conferences.

	2024 €	2023 €
Support costs comprise:		
Bank charges	844	814
Donated services	37,364	37,364
Other support costs	618	4,455
	38,826	42,633

It is estimated that the charity benefited from approximately 636 (2023: 636) hours of donated time provided to assist with the running of the charity. This figure was made up of 477 (2023: 477) hours of donated time received as a contribution in kind from the CCP9 service level agreement, and 159 (2023: 159) hours from the Science and Technology Facilities Council.

5. GOVERNANCE COSTS

	Total 2024 €	Total 2023 €
Governance costs are made up of the following:		
Independent examiners fee	4,917	4,487
Accountancy	6,704	6,457
	11,622	10,944

6. STAFF COSTS

There were no employees in the year.

The Trustees were not paid any remuneration and so there is no remuneration paid to key management personnel. No expenses were incurred or reimbursed during the year (2023: Nil).

PSI-K
NOTES TO THE FINANCIAL STATEMENTS
YEAR ENDED 31 DECEMBER 2024

7. TAXATION

PSI-K is a registered charity and is therefore exempt from tax on its charitable income.

8. GRANTS MADE TO INSTITUTIONS	2024		2023	
	€	€	€	€
Grants awarded in the year were all to institutions and comprised:				
CECAM, Lausanne	26,600		19,750	
ICTP Trieste (Italy)	-		25,000	
Alto University, Helsinki, Finland	3,600		6,000	
Benasque Science Centre, Benasque, Spain	10,000		-	
ICN2, Barcelona Area, Spain	4,050		-	
Liège, Belgium	7,200		-	
Indian Institute of Science Education and Research, India	8,000		-	
SISSA, Trieste, Italy	8,000		-	
University of Zadar, Zadar, Croatia	5,000		-	
Berlin, Germany			6,000	
Dresden University of Technology, Dresden, Germany	4,050		-	
Gandía and University of Valencia, Spain	4,800		-	
Forschungszentrum Jülich, Jülich, Germany	7,000		-	
Modena, Italy	9,000		-	
University of Tokyo, Hongo Campus	8,400		-	
Albert-Ludwigs-Universität Freiburg, Germany	-		3,000	
London, UK	-		8,900	
Science Technology Park Belgrade, Belgrade, Serbia	4,500		-	
University of Siena, Piazza San Francesco n.7, Siena	7,500		-	
Budapest, Hungary	4,000		-	
Toulouse, France	-		6,000	
Marseille, France	-		6,000	
Jožef Stefan Institute, Ljubljana, Slovenia	-		6,000	
Eötvös University, Budapest, Hungary	-		6,000	
Durham, UK	-		5,000	
Leipzig (Online)	-		2,400	
Max Planck Institute for Polymer Research, Mainz, Germany	-		5,400	
Vienna, Austria	-		6,000	
Total institutional grants	121,700		111,450	
Reconciliation of grants payable				
Grant commitments brought forward		171,005		160,990
Commitments made during the year	121,700		111,450	
Grant commitments for the year	121,700		111,450	
Grants payable for the year (note 4)		121,700		111,450
Grants paid during the year		(100,796)		(101,435)
Grant commitments carried forward		191,909		171,005

These unaudited financial statements have been subjected to independent examination. See report on page 8.

PSI-K
NOTES TO THE FINANCIAL STATEMENTS
YEAR ENDED 31 DECEMBER 2024

9. DEBTORS	2024	2023
	€	€
Trade debtors	21,629	28,038
Accrued income	-	2,863
	21,629	30,901
10. CREDITORS: Amounts falling due within one year	2024	2023
	€	€
Grant commitments	191,909	171,005
Accruals	11,323	10,700
Deferred income	32,000	-
	235,232	181,705

11. STATEMENT OF FUNDS

The movements on the funds of the charity were as follows:

	Balance 01.01.24	Income	Expenditure	Transfer	Balance 31.12.24
	€	€	€	€	€
Unrestricted Funds					
General Fund	372,102	149,499	(172,008)	-	349,593
	372,102	149,499	(172,008)	-	349,593
Total Funds					
	372,102	149,499	(172,008)	-	349,593

The movement on the funds of the charity in 2023 were as follows:

	Balance 01.01.23	Income	Expenditure	Transfer	Balance 31.12.23
	€	€	€	€	€
Unrestricted Funds					
General Fund	414,931	122,216	(165,045)	-	372,102
	414,931	122,216	(165,045)	-	372,102
Total Funds					
	414,931	122,216	(165,045)	-	372,102

All funds for the year ended 31 December 2024 and year ended 31 December 2023 relate to unrestricted reserves.

PSI-K
NOTES TO THE FINANCIAL STATEMENTS
YEAR ENDED 31 DECEMBER 2024

12. ANALYSIS OF NET ASSETS BETWEEN FUNDS

	Unrestricted Funds €	Total 2024 €
Fund balances at 31 December 2024 are represented by:		
Current assets	584,825	584,825
Creditors: Amounts falling due within one year	(235,232)	(235,232)
Total Net Assets	<u>349,593</u>	<u>349,593</u>
	Unrestricted Funds €	Total 2023 €
Fund balances at 31 December 2023 are represented by:		
Current assets	553,807	553,807
Creditors: Amounts falling due within one year	(181,705)	(181,705)
Total Net Assets	<u>372,102</u>	<u>372,102</u>

13. GUARANTEE COMPANY AND LIABILITY OF MEMBERS

Psi-k is a company limited by guarantee and therefore does not have any share capital.

The liability of members is limited. In the event of the charity being wound up during a member's period of membership or within one year after ceasing to be a member, an amount not exceeding the sum of £1 may be required from that member towards the payment of the debts and liabilities of the company incurred before membership ceased and the costs of winding up.

At 31 December 2024, the company had 11 (2023: 9) members.

14. RELATED PARTY

There are deemed to be no related parties of the entity which require reporting during the year (2023: none).

PSI-K

England & Wales - Charity number 1126308

Accounts

Company registration number 06440198
Charity Commission number 1126308

PSI-K
(A company limited by guarantee)

REPORT AND UNAUDITED FINANCIAL STATEMENTS

YEAR ENDED 31 DECEMBER 2023

PSI-K
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**PSI-K
LEGAL AND ADMINISTRATIVE INFORMATION
YEAR ENDED 31 DECEMBER 2023**

Psi-k is a company limited by guarantee and a registered charity governed by its Memorandum and Articles of Association dated 29 November 2007.

Company registration number: 06440198

Charity registration number: 1126308

DIRECTORS AND TRUSTEES

The directors of the company are its Trustees for the purpose of Charity Law and throughout this report are collectively referred to as the Trustees. The Trustees who served during the period and to the date of this report are set on page 4.

SECRETARY

Damian Jones

REGISTERED AND PRINCIPAL OFFICE

Stfc Scitech Daresbury
Daresbury
Warrington
Cheshire
WA4 4AD

ACCOUNTANTS & INDEPENDENT EXAMINERS

RSM UK Tax and Accounting Limited
Chartered Accountants
The Pinnacle
170 Midsummer Boulevard
Milton Keynes
Buckinghamshire
MK9 1BP

BANKERS

HSBC Bank Plc
11 Stamford New Road
Altrincham
Cheshire
WA14 1BW

**PSI-K
REPORT OF THE CHAIRMAN
YEAR ENDED 31 DECEMBER 2023**

In 2023, the Psi-k Charity supported a diverse and stimulating scientific and educational programme of 25 workshops, summer schools and hands-on tutorials, the list of which can be found at <https://psi-k.net/psi-k-workshops/>. Among these were: the major annual research conference supported jointly with CECAM, the European Centre for Atomic and Molecular Calculations (CECAM), on the topic of Bridging length scales with machine learning: from wavefunctions to thermodynamics (<https://sites.google.com/view/cecam-psik-2023/home>); schools and tutorials aimed specifically at training graduate students and early career researchers in state-of-the-art methods in computational materials science and related subjects, including the Young Researchers' School on Theory and Simulation in Electrochemical Conversion Processes (<https://www.cecarn.org/workshop-details/1216>), and the School on Machine Learning Interatomic Potentials (<https://www.cecarn.org/workshop-details/1213>); and the first event that we have supported in India, New approaches and machine learning methods for ab initio calculations (<https://nammapsik.iisc.ac.in>).

One Psi-k Highlight was published in October on "CELL: a Python package for cluster expansion with a focus on complex alloys" by Santiago Rigamonti, Maria Troppenz, Martin Kuban, Axel Huebner, and Claudia Draxl, and can be found at <https://psi-k.net/highlights/>, together with all those published from 1994 onwards. The Highlight series showcases work that combines breadth and depth and is relevant to the Psi-k community. Suggested contributions can be discussed with leon.petit@stfc.ac.uk. We have established informal agreements with journals including npj Computational Materials and IOP Electronic Structure that provide opportunities for open-access publication of Psi-k Highlights.

We continue to be inspired by the generous donations by groups worldwide, which enable Psi-k's rich programme of activities. In 2023, 25 groups or institutions from 12 countries contributed to the charity. Anyone (individuals, groups, organisations, companies) who would like to contribute may contact a.mostofi@imperial.ac.uk and PSIK_ADMIN@stfc.ac.uk, or contribute directly using PayPal via the link at <https://psi-k.net>.

2023 has also seen a full refresh of PSI-K's Working Groups, which were last reorganised in 2017. This refresh was informed both by the topical distribution of abstracts in the 2022 Psi-k Conference in Lausanne, and through direct community engagement. It has resulted in a total of 22 Working Groups (up from 16 previously), organised by four main themes (up from three previously), each overseen by at least one Trustee (named in parenthesis):

- A. Physical formalisms – Lucia Reining and (Silke Biermann)
- B. Algorithms, software and data – Arash Mostofi and (Stefan Blügel)
- C. Applications to real materials and materials design – (Igor Abrikosov) and (Elisa Molinari)
- D. Wider engagement – (Nicola Marzari) and (Peter Haynes)

In addition to the scientific topics covered in themes A to C, the new theme D includes Working Groups dedicated to social responsibility, early career researchers, industry engagement, training and education, and policy engagement. As of the end of 2023, the membership of the Working Groups is being finalised to be ready for the 2024 cycle of proposals for activities. Further information about the Working Groups can be found at <https://psi-k.net/groups/>.

The Working Groups are instrumental in soliciting proposals for activities from the community, and assisting Trustees in evaluating proposals submitted in a two-step process: there is a first deadline at the end of July for outline proposals; these are evaluated and either encouraged to submit a full proposal by the end of October, rejected right away, or advised to merge with other efforts on similar themes to avoid duplication. The Psi-k/CECAM Research Conference has a separate track, and proposals not selected but deemed of sufficient quality can directly apply as a full proposal.

**PSI-K
REPORT OF THE CHAIRMAN (Continued)
YEAR ENDED 31 DECEMBER 2023**

The Board of Trustees met five times in 2023, all by teleconference: on 17 February, 21 April, 23 June, 15 September and 3 November. Minutes of meetings are recorded, circulated, and kept for internal use. The Trustees (<https://psi-k.net/admin/>), plus Working Group leaders (<https://psi-k.net/groups/>) and members of the Scientific Advisory Committee (<https://psi-k.net/scientific-advisory-committee/>) attended the Annual Meeting on 24 November, where all activities are finalised for the following year (in this case, from April 2024 to March 2025).

The generous contribution of time from all the groups above is essential to the wellbeing of the charity, but particular thanks must go to our Operations Manager, Damian Jones, (STFC Daresbury Laboratory, UK) for coordinating all the administration; to Igor Abrikosov and Nicola Marzari, who stepped down as a Trustees at the end of 2023, having served for 10 and 12 years, respectively; and to Peter Haynes who stepped down as Psi-k Chair, having served his three-year tenure, and who remains a Trustee and will Chair the next Psi-k Conference in 2025.



Arash Mostofi - Psi-K Chair

Date: 28/10/24

**PSI-K
REPORT OF THE TRUSTEES
YEAR ENDED 31 DECEMBER 2023**

The Trustees present their annual report and unaudited financial Statements for the year ended 31 December 2023.

Trustees

The Trustees who served during the period and to the date of this report were:

*Igor Abrikosov
Silke Biermann
Stefan Blügel
Claudia Draxl
Martin Friak
Peter Haynes (resigned as Chair)
*Nicola Marzari
Angelos Michaelides
Elisa Molinari
Arash Mostofi (appointed as Chair)
Lucia Reining

The Trustee whose name are starred (*) resigned following the Annual Meeting on 24 November 2023.

Structure, governance and management

The organisation is governed by its Memorandum and Articles of Association and is a registered company limited by guarantee.

Psi-k is a Europe-based, worldwide network of researchers working on the advancement of first-principles computational materials science. Its mission is to develop fundamental theory, algorithms, and computer codes in order to understand, predict, and design materials properties and functions. Theoretical condensed matter physics, quantum chemistry, thermodynamics, and statistical mechanics form its scientific core. Applications encompass inorganic, organic and bio-materials, and cover a whole range of diverse scientific, engineering, and industrial endeavours. Key activities of Psi-k are the organisation of conferences, workshops, tutorials and training schools as well as the dissemination of scientific thinking in society.

Psi-k has a minimum of three Trustees, but there is no maximum. On the date of this report there were nine Trustees.

Psi-k has a Chair, and a Scientific Advisory Committee (SAC) of about 80 members, which is headed by the Chair of Psi-k. In addition all Trustees are also SAC members.

The Board of Trustees meets on average five to six times a year, normally with a combination of face-to-face meetings and teleconference meetings. In 2023 there were five meetings, all by teleconference: on 17 February, 21 April, 23 June, 15 September and 3 November. The Trustees had the opportunity to meet in person at the Annual Meeting of the SAC on 24 November. Minutes of meetings are recorded, circulated, and kept for internal use. The Board of Trustees uses these meetings to discuss matters including but not limited to: future strategy, funding and finances, events such as workshops, conferences and summer schools, and relationships with external organisations such as CECAM.

The day to day running of Psi-k is delegated to the Chair, Peter Haynes, who resigned with effect from 31 December but remains a Trustee. The Chair from 1 Jan 2024 is Arash Mostofi. The Chair is supported by the Operations Manager, Damian Jones.

The SAC meets once a year, normally in November, together with the leaders of the 16 Working Groups (<https://psi-k.net/groups/>). It is chaired by the Chair of Psi-k and its role is to make recommendations to the Board of Trustees, particularly regarding plans for all activities for the following year (in this case, from April 2024 to March 2025). In 2023 the Annual Meeting was held on 24 November in hybrid mode: in person in Paris and online.

PSI-K
REPORT OF THE TRUSTEES (Continued)
YEAR ENDED 31 DECEMBER 2023

All Trustees gave their time freely and no Trustee remuneration was paid in the year: expenses paid to Trustees amounted to €nil. Trustees are required to disclose all relevant interests and register them with the Chair.

Trustees are required to declare any conflicts of interest at each meeting and these are recorded in the minutes. If a vote of the Trustees is required on a matter, a Trustee who has declared a conflict of interest on that matter may not cast a vote.

Risk management

The Trustees have considered the major risks to which the charity is exposed and have reviewed those risks and established systems and procedures to manage those risks.

A significant risk for the Psi-k Charity is reduced financial funding. Since 2016, Psi-k has been sustained entirely by donations. In 2021 the Trustees agreed that our annual expenditure on community activities is determined by our income from the previous year, and adopted a target for reserves of €200,000.

Objectives and activities

Europe has become the leading research area in the world for the application of first-principles computational modelling to materials science and Psi-k aims to maintain and enhance this status.

“Psi-k research” covers structures, properties and processes in all types of materials at the atomic level and in nanometre-scale structures, studied by *ab initio* quantum-mechanical computer simulation. A series of working groups represent the views of the community and organise activities to deliver the Psi-k mission. During 2023 these were refreshed to reflect current trends in the discipline and to expand their scope with the creation of a new Theme D:

Theme A: Physical Formalisms: Ground State and Spectroscopy of Many-Electron Systems	
WG A1	Density and density-matrix functional theories
WG A2	Perturbative many-body methods
WG A3	Non-perturbative many-body methods
WG A4	Open and non-equilibrium systems
WG A5	Phonons, electron-phonon coupling and related phenomena
Theme B: Algorithms, Software and Data	
WG B1	Multiscale and reduced-scaling methods
WG B2	Statistics and configuration sampling
WG B3	Software engineering
WG B4	High-throughput workflows and data analytics
WG B5	Artificial intelligence methods for materials genomics
Theme C: Applications to Real Materials and Materials Design	
WG C1	Structural materials
WG C2	Materials and devices for energy
WG C3	Quantum materials driven by correlations, topology or spin
WG C4	Catalysis and electrochemistry
WG C5	Materials for information and communication
WG C6	Nanoscale structures (2D, 1D, 0D) and related phenomena
WG C7	Molecules, macromolecules and biomolecules
Theme D: Wider Engagement	
WG B1	Social responsibility
WG B2	Early career researchers
WG B3	Industry engagement
WG B4	Training and education
WG B5	Policy engagement

PSI-K
REPORT OF THE TRUSTEES (Continued)
YEAR ENDED 31 DECEMBER 2023

Psi-k will promote and coordinate collaboration within the European research community by, among others, the following measures:

- supporting workshops and small conferences on specific topics of active research;
- supporting summer schools, tutorial courses and other training activities for early career and new researchers in the field;
- organising a large “Psi-k conference” every few years (such as those previously held in 1996, 2000, 2005, 2010, 2015 and 2022): the next one is planned for 2025.
- disseminating information about research progress, job opportunities, relevant workshops, conferences and other events, and funding opportunities via the Psi-k website, providing a portal and a newsletter available freely to anyone in the world by electronic means.

The activities are open to all researchers in the field. Psi-k acts as a vehicle to engaging with the wider scientific community, with industry, European policy makers and trans-European computer centres. It will seek to maintain cooperation with organisations such as the Centre Européen de Calcul Atomique et Moléculaire (CECAM), the European molecular simulation community and its networks and Psi-k’s counterpart research communities on other continents.

Aims and objectives for 2023

The main activities planned during 2023 comprised the scientific programme of workshops, tutorials and summer schools on the electronic structure of complex processes in materials, i.e. the topic of the Psi-k Charity. The programme comprised 25 events, including the major annual research conference supported jointly with CECAM, the European Centre for Atomic and Molecular Calculations (CECAM), on the topic of “Bridging length scales with machine learning: from wavefunctions to thermodynamics” (<https://sites.google.com/view/cecam-psik-2023/home>).

Grant making policy

The Psi-k Charity does not make grants to other research bodies. Generally, grant payments are made to institutions regarding scientific conferences.

The Psi-k Charity applies its funding to the organization of workshops, summer schools, hands-on courses and the Psi-k Conference. The Theoretical and Computational Physics Group at STFC Daresbury Laboratory publishes the Psi-k Newsletter and provides administrative support.

The achievements of every workshop to which Psi-k contributes are monitored in the form of a report which is published on the Psi-k website (<http://psi-k.net/>).

Key performance indicators

In 2023 the Psi-k Charity organised 25 workshops, conferences and training activities, which is in the middle of the typical range of 20 to 25 events and activities that have been supported in previous years.

Financial review 2023 and plan for 2024

Unrestricted net expenditure for the year was (€42,829) (2022: net income of €75,976). Unrestricted retained funds at the year end were €372,102 (2022: €414,931).

Member donations in 2023 amounted to a total of about €100,000 received. The expenses in the 2023 budget included €120,000 for workshops.

Plan for 2024: The Trustees continue to seek new contributors with an aim of increasing annual donations to around €150,000. The amount of €121,000 will be spent for workshops in 2024. Any deficit will be covered by the reserves.

During the year 2023 the Trustees were satisfied that, as far as circumstances permitted, the Charity continued to benefit the public through its activities targeted to achieve its charitable objectives.

Public Benefit

The Trustees confirm that they have referred to the guidance contained in the Charity Commission’s general guidance on public benefit when reviewing the Trust’s aims and objectives and in planning future activities and setting the grant making policy for the year.

PSI-K
REPORT OF THE TRUSTEES (Continued)
YEAR ENDED 31 DECEMBER 2023

Trustees' responsibilities

The Trustees (who are also Directors of Psi-k for the purposes of company law) are responsible for preparing the Trustees' Annual Report and the financial statements in accordance with applicable law and United Kingdom Accounting Standards (United Kingdom Generally Accepted Accounting Practice).

Company Law requires the Trustees to prepare financial statements for each financial year which give a true and fair view of the state of affairs of the charitable company and of the incoming resources and applications of resources, including the income and expenditure, of the charitable company for that year. In preparing those financial statements, the Trustees are required to:

- provide statements on the going concern basis unless it is inappropriate to presume that the charitable company will continue in business;
- select suitable accounting policies and apply them consistently;
- observe the methods and principles in the Charitable SORP;
- make judgements and estimates that are reasonable and prudent;
- state whether applicable accounting standards have been followed, subject to any material departures disclosed and explained in the financial statements.

The Trustees are responsible for keeping proper accounting records that disclose with reasonable accuracy at any time the financial position of the charitable company and enable them to ensure that the financial statements comply with the Companies Act 2006. They are also responsible for safeguarding the assets of the charitable company and hence for taking reasonable steps for the prevention of fraud and other irregularities.

This report has been prepared in accordance with the Statement of Recommended Practice: Accounting and Reporting by Charities (issued in October 2019) and in accordance with the special provisions applicable to small companies.

ON BEHALF OF THE BOARD



Arash Mostofi (Chair)

Date: 28/10/24

INDEPENDENT EXAMINER'S REPORT TO THE TRUSTEES OF PSI-K

I report to the trustees on my examination of the financial statements of PSI-K ("the company") for the year ended 31 December 2023, which are set out on pages 9 to 16.

Responsibilities and basis of report

As the trustees of the company (and also its directors for the purposes of company law) you are responsible for the preparation of the financial statements in accordance with the requirements of the Companies Act 2006 ('the 2006 Act').

Having satisfied myself that the financial statements of the company are not required to be audited under Part 16 of the 2006 Act and are eligible for independent examination I report in respect of my examination of your charity's financial statements as carried out under section 145 of the Charities Act 2011 ('the 2011 Act'). In carrying out my examination I have followed the Directions given by the Charity Commission under section 145 (5)(b) of the 2011 Act.

An independent examination does not involve gathering all the evidence that would be required in an audit and consequently does not cover all the matters that an auditor considers in giving their opinion on the financial statements. The planning and conduct of an audit goes beyond the limited assurance that an independent examination can provide. Consequently, I express no opinion as to whether the financial statements present a 'true and fair view' and my report is limited to those specific matters set out in the independent examiner's statement.

Independent examiner's statement

I have completed my examination. I confirm that no material matters have come to my attention in connection with the examination giving me reasonable cause to believe that in any material respect:

1. accounting records were not kept in respect of the company as required by section 386 of the 2006 Act; or
2. the financial statements do not accord with those records; or
3. the financial statements do not comply with the accounting requirements of section 396 of the 2006 Act other than any requirement that the financial statements give a 'true and fair view' which is not a matter considered as part of an independent examination; or
4. the financial statements have not been prepared in accordance with the methods and principles of the Statement of Recommended Practice: Accounting and Reporting by Charities applicable to charities preparing their financial statements in accordance with the Financial Reporting Standard applicable in the UK and Ireland (FRS 102).

I have no concerns and have come across no other matters in connection with the examination to which attention should be drawn in this report in order to enable a proper understanding of the financial statements to be reached.

S Monteith

Name: **Sharon Monteith**

Name of applicable listed body: **The Institute of Chartered Accountants in England and Wales**

Relevant professional qualification or membership of professional body: **Chartered Accountant**

ON BEHALF OF RSM UK TAX AND ACCOUNTING LIMITED

Chartered Accountants
The Pinnacle
170 Midsummer Boulevard
Milton Keynes
Buckinghamshire
MK9 1BP
Date: 28/10/24

PSI-K
STATEMENT OF FINANCIAL ACTIVITIES
INCLUDING INCOME AND EXPENDITURE ACCOUNT
YEAR ENDED 31 DECEMBER 2023

	Notes	Unrestricted Funds €	Total Funds 2023 €	Total Funds 2022 €
INCOME				
Donations and legacies				
- Donated services		37,364	37,364	37,364
Charitable activities				
- Donations from research bodies		84,852	84,852	101,499
TOTAL INCOME		<u>122,216</u>	<u>122,216</u>	<u>138,863</u>
EXPENDITURE				
Charitable activities	4	165,045	165,045	62,887
TOTAL EXPENDEDITURE		<u>165,045</u>	<u>165,045</u>	<u>62,887</u>
NET (EXPENDITURE)/INCOME AND NET MOVEMENT IN FUNDS FOR THE YEAR		<u>(42,829)</u>	<u>(42,829)</u>	<u>75,976</u>
RECONCILIATION OF FUNDS				
TOTAL FUNDS BROUGHT FORWARD		<u>414,931</u>	<u>414,931</u>	<u>338,955</u>
TOTAL FUNDS CARRIED FORWARD	12	<u><u>372,102</u></u>	<u><u>372,102</u></u>	<u><u>414,931</u></u>

The statement of financial activities includes all gains and losses recognised in the year.

All income and expenditure derive from continuing activities and are attributed to unrestricted funds.

The statement of financial activities also complies with the requirements for an income and expenditure account under the Companies Act 2006.

**PSI-K
BALANCE SHEET
AS AT 31 DECEMBER 2023**

Company registration number 06440198

	Notes	2023 €	2022 €
CURRENT ASSETS			
Debtors	9	30,901	150,583
Cash at bank		522,906	433,267
		<u>553,807</u>	<u>583,850</u>
CURRENT LIABILITIES			
CREDITORS: Amounts falling due within one year	10	(181,705)	(168,919)
		<u></u>	<u></u>
NET CURRENT ASSETS		<u>372,102</u>	<u>414,931</u>
INCOME FUNDS			
Unrestricted funds	12	372,102	414,931
Restricted funds	12	-	-
		<u></u>	<u></u>
	12	<u>372,102</u>	<u>414,931</u>

For the year ending 31 December 2023 the company was entitled to exemption from audit under Section 477 of the Companies Act 2006 relating to small companies.

The members have not required the company to obtain an audit of its financial statements for the year ended 31 December 2023 in accordance with Section 476 of the Companies Act 2006.

The directors acknowledge their responsibilities for:

- ensuring that the company keeps accounting records which comply with Section 396 of the Companies Act 2006; and
- preparing financial statements which give a true and fair view of the state of affairs of the company as at the end of each financial year and of its profit or loss for each financial year in accordance with the requirements of Section 396 and which otherwise comply with the requirements of the Companies Act 2006 relating to financial statements, so far as applicable to the company.

These financial statements are prepared in accordance with the provisions applicable to companies subject to the small companies regime and in accordance with Charities SORP (FRS102).

The notes on pages 11 to 16 form part of these financial statements.

The financial statements were approved by the Trustees and authorised for issue on 28/10/24..... and were signed on their behalf by:



Arash Mostofi (Chair)

Trustee

These unaudited financial statements have been subjected to independent examination. See report on page 8.

PSI-K
NOTES TO THE FINANCIAL STATEMENTS
YEAR ENDED 31 DECEMBER 2023

1. ACCOUNTING POLICIES

a. Basis of preparation

The financial statements have been prepared in accordance with Accounting and Reporting by Charities: Statement of Recommended Practice applicable to charities preparing their financial statements in accordance with the Financial Reporting Standard applicable in the UK and Republic of Ireland (FRS 102) (Issued October 2019) - (Charities SORP (FRS 102)), the Financial Reporting Standard applicable in the UK and Republic of Ireland (FRS 102) and the Companies Act 2006.

The financial statements are prepared in Euro and amounts in these financial statements are rounded to the nearest Euro.

PSI-K meets the definition of a public benefit entity under FRS 102. Assets and liabilities are initially recognised at historical cost or transaction value unless otherwise stated in the relevant accounting policy notes.

b. Preparation of the financial statements on a going concern basis

The trustees forecast that the charity will continue to be able to pay its liabilities as they fall due for a period of at least 12 months following the date of approving the financial statements. The forecasts take into account transactions that are anticipated to take place in the foreseeable future and indicate that no additional financial resources will be required should the actual performance differ from forecast. On this basis the trustees have concluded that adopting the going concern basis of accounting in preparing the annual financial statements is appropriate.

c. Income recognition

Incoming resources represents donations from research bodies in Europe to support the company's activities, less amounts carried forward to future periods as deferred income; and donated services, which are included based on the hours worked and the appropriate hourly rate. Income is recognised when the entity has entitlement to the funds, it is probable that the income will be received and the amount can be measured reliably.

d. Donated services

Donated services are included within incoming resources with an equivalent amount shown within resources expended, where the benefit to the charity is reasonably quantifiable, measurable and material. The value placed on these resources is the estimated value to the charity of the service received.

e. Deferred income

Donations received in advance of the period that they relate to, or which are provided specifically for future periods, are carried forward as deferred income. These amounts relate to contributions from research bodies received in advance.

f. Expenditure recognition

All expenditure is accounted for on an accruals basis, inclusive of any VAT which cannot be recovered.

Grants payable are payments made to third parties in the furtherance of the charitable objectives of the Charity. Grants are accounted for when either the recipient has a reasonable expectation that they will receive a grant and the trustees have agreed to pay the grant without condition, or the recipient has a reasonable expectation that they will receive a grant and any condition attaching to the grant is outside of the control of the Charity.

Provisions for grants are made when the intention to make a grant has been communicated to the recipient but there is uncertainty about either the timing of the grant or the amount of grant payable.

Governance costs are related to the governance of the charity, such as the costs of preparing the financial statements and statutory compliance.

Irrecoverable VAT is charged as a cost against the activity for which the expenditure was incurred.

PSI-K
NOTES TO THE FINANCIAL STATEMENTS
YEAR ENDED 31 DECEMBER 2023

1. ACCOUNTING POLICIES (Continued)

g. Charitable Funds

Restricted funds are to be used for specified purposes as laid down by the donor. Expenditure which meets these criteria is identified to the fund, together with a fair allocation of management and support costs.

Unrestricted funds are available for use at the discretion of the Trustees in furtherance of the general objectives of the Charity.

h. Foreign currencies

The trustees consider that the functional currency of the charity is the Euro, as most transactions are denominated and are carried out in that currency.

Assets and liabilities denominated in other currencies are translated into Euros at the rate of exchange ruling at the balance sheet date. Transactions in other currencies are translated into Euros at the rate of exchange ruling at the date of the transaction. Exchange differences are taken into account in arriving at the net movement in funds in the Statement of Financial Activities.

At the balance sheet date the rate of exchange between Sterling and Euro was £1 equals €1.1505 (2022: €1.1295).

i. Financial instruments

The Charity has elected to apply the provisions of Section 11 'Basic Financial Instruments' and Section 12 'Other Financial Instruments Issues' of FRS 102, in full, to all of its financial instruments.

Financial assets and financial liabilities are recognised when the Charity becomes a party to the contractual provisions of the instrument, and are offset only when the Charity currently has a legally enforceable right to set off the recognised amounts and intends either to settle on a net basis, or to realise the asset and settle the liability simultaneously.

j. Basic Financial assets

Trade and other debtors (including accrued income) which are receivable within one year and which do not constitute a financing transaction are initially measured at the transaction price and subsequently measured at amortised cost, being the transaction price less any amounts settled and any impairment losses.

k. Basic Financial liabilities

Financial instruments are classified as liabilities according to the substance of the contractual arrangements entered into.

Trade and other creditors (including accruals) payable within one year that do not constitute a financing transaction are initially measured at the transaction price and subsequently measured at amortised cost, being the transaction price less any amounts settled.

l. Derecognition of financial liabilities

Financial liabilities are derecognised when the charity's contractual obligations expire or are discharged or cancelled

2. CRITICAL ACCOUNTING ESTIMATES AND JUDGMENT

In the application of the Charity's accounting policies, the trustees are required to make judgements, estimates and assumptions about the carrying amount of assets and liabilities that are not readily apparent from other sources. The estimates and associated assumptions are based on historical experience and other factors that are considered to be relevant. Actual results may differ from these estimates.

The estimates and underlying assumptions are reviewed on an on-going basis. Revisions to accounting estimates are recognised in the period in which the estimate is revised where the revision affects only that period, or in the period of the revision and future periods where the revision affects both current and future periods.

No critical accounting estimates and judgements have been made in preparing these financial statements.

PSI-K
NOTES TO THE FINANCIAL STATEMENTS
YEAR ENDED 31 DECEMBER 2023

3. INCOME

Donations received from research bodies attributable to overseas markets total **96%** (2022: 96%). All income received in 2023 (and 2022) was unrestricted.

4. TOTAL EXPENDITURE

	Grant Funding of Activities €	Support Costs €	Total 2023 €	Total 2022 €
Charitable Activities				
Grants payable	111,450	-	111,450	5,860
Support costs	-	42,633	42,633	41,886
Prize giving awards and donations	-	-	-	6,500
Exchange losses	-	18	18	517
Governance Costs (Note 5)	-	10,944	10,944	8,124
	<u>111,450</u>	<u>53,595</u>	<u>165,045</u>	<u>62,887</u>

Total expenditure for the year was €165,045, all of which was unrestricted expenditure (2022: €62,887).

The grant funding of activities totalling €111,450 (2022: €5,860) relates to payments made to institutions regarding scientific conferences.

	2023 €	2022 €
Support costs comprise:		
Bank charges	814	521
Donated services	37,364	37,364
Other support costs	4,455	4,001
	<u>42,633</u>	<u>41,886</u>

It is estimated that the charity benefited from approximately 636 (2022: 636) hours of donated time provided to assist with the running of the charity. This figure was made up of 477 (2022: 477) hours of donated time received as a contribution in kind from the CCP9 service level agreement, and 159 (2022: 159) hours from the Science and Technology Facilities Council.

5. GOVERNANCE COSTS

	Total 2023 €	Total 2022 €
Governance costs are made up of the following:		
Independent examiners fee	4,487	3,863
Accountancy	6,457	4,261
	<u>10,944</u>	<u>8,124</u>

6. STAFF COSTS

There were no employees in the year.

The Trustees were not paid any remuneration and so there is no remuneration paid to key management personnel. No expenses were incurred or reimbursed during the year (2022: Nil).

PSI-K
NOTES TO THE FINANCIAL STATEMENTS
YEAR ENDED 31 DECEMBER 2023

7. TAXATION

PSI-K is a registered charity and is therefore exempt from tax on its charitable income.

8. GRANTS MADE TO INSTITUTIONS	2023		2022	
	€	€	€	€
Grants awarded in the year were all to institutions and comprised:				
CECAM, Lausanne	19,750		13,500	
ICTP Trieste (Italy)	25,000		16,500	
Alto University, Helsinki, Finland	6,000		12,050	
STFC Rutherford Appleton Laboratory, UK	-		4,000	
Forschungszentrum Julich, Germany	-		2,500	
Rome, Italy	-		3,750	
Ecole Normale Supérieure, Paris, France	-		6,000	
CECAM-ISR, Tel Aviv University, Israel	-		4,000	
Zaragoza, Spain	-		6,000	
Berlin, Germany	6,000		20,000	
Modena	--		4,500	
Bangalore, India	--		5,000	
Orebro, Sweden	-		5,000	
University of Pavia, Italy	-		5,000	
Athens, Greece	-		4,000	
Albert-Ludwigs-Universität Freiburg, Germany	3,000		3,600	
London, UK	8,900		3,000	
National Graphene Institute, Manchester UK	-		3,000	
Paphos, Cyprus	-		5,000	
Reingberg, Tegernsee, Germany	-		5,000	
Les Houches School of Physics, France	-		6,000	
Toulouse, France	6,000		-	
Marseille, France	6,000		-	
Jožef Stefan Institute, Ljubljana, Slovenia	6,000		-	
Eötvös University, Budapest, Hungary	6,000		-	
Durham, UK	5,000		-	
Leipzig (Online)	2,400		-	
Max Planck Institute for Polymer Research, Mainz, Germany	5,400		-	
Vienna, Austria	6,000		-	
Total institutional grants	111,450		137,400	
Reconciliation of grants payable				
Grant commitments brought forward		160,990		154,034
Commitments made during the year	111,450		137,400	
Grant commitments for the year	111,450		137,400	
Grants cancelled, recovered or refunded	-		(131,540)	
Grants payable for the year (note 4)		111,450		5,860
Grants paid during the year		(101,435)		(98,904)
Grants to be refunded post year end transferred to other debtors (note 9)		-		100,000
Grants refunded in the year		-		-
Grant commitments carried forward		171,005		160,990

These unaudited financial statements have been subjected to independent examination. See report on page 8.

PSI-K
NOTES TO THE FINANCIAL STATEMENTS
YEAR ENDED 31 DECEMBER 2023

9. DEBTORS	2023	2022
	€	€
Trade debtors	28,038	40,583
Accrued income	2,863	10,000
Other debtors	-	100,000
	30,901	150,583
10. CREDITORS: Amounts falling due within one year	2023	2022
	€	€
Grant commitments	171,005	160,990
Accruals	10,700	7,929
Deferred income (note 11)	-	-
	181,705	168,919
11. DEFERRED INCOME	2023	2022
	€	€
Deferred income as at 1 January	-	7,000
Received in year	-	-
Released in year	-	(7,000)
Deferred income as at 31 December	-	-

Deferred income comprises contributions from research bodies received pre 31 December 2023 which have been invoiced in advance.

12. STATEMENT OF FUNDS

The movements on the funds of the charity were as follows:

	Balance 01.01.23	Income	Expenditure	Transfer	Balance 31.12.23
	€	€	€	€	€
Unrestricted Funds					
General Fund	414,931	122,216	(165,045)	-	372,102
	414,931	122,216	(165,045)	-	372,102
Total Funds	414,931	122,216	(165,045)	-	372,102

These unaudited financial statements have been subjected to independent examination. See report on page 8.

PSI-K
NOTES TO THE FINANCIAL STATEMENTS
YEAR ENDED 31 DECEMBER 2022

12. STATEMENT OF FUNDS (continued)

The movement on the funds of the charity in 2022 were as follows:

	Balance 01.01.22	Income	Expenditure	Transfer	Balance 31.12.22
	€	€	€	€	€
Unrestricted Funds					
General Fund	338,955	138,863	(62,887)	-	414,931
	<u>338,955</u>	<u>138,863</u>	<u>(62,887)</u>	<u>-</u>	<u>414,931</u>
Total Funds	<u>338,955</u>	<u>138,863</u>	<u>(62,887)</u>	<u>-</u>	<u>414,931</u>

All funds for the year ended 31 December 2023 and year ended 31 December 2022 relate to unrestricted reserves.

13. ANALYSIS OF NET ASSETS BETWEEN FUNDS

	Unrestricted Funds €	Total 2023 €
Fund balances at 31 December 2023 are represented by:		
Current assets	553,807	553,807
Creditors: Amounts falling due within one year	(181,705)	(181,705)
Total Net Assets	<u>372,102</u>	<u>372,102</u>
	Unrestricted Funds €	Total 2022 €
Fund balances at 31 December 2022 are represented by:		
Current assets	583,850	583,850
Creditors: Amounts falling due within one year	(168,919)	(168,919)
Total Net Assets	<u>414,931</u>	<u>414,931</u>

14. GUARANTEE COMPANY AND LIABILITY OF MEMBERS

Psi-k is a company limited by guarantee and therefore does not have any share capital.

The liability of members is limited. In the event of the charity being wound up during a member's period of membership or within one year after ceasing to be a member, an amount not exceeding the sum of £1 may be required from that member towards the payment of the debts and liabilities of the company incurred before membership ceased and the costs of winding up.

At 31 December 2023, the company had 9 (2022: 10) members.

15. RELATED PARTY

There are deemed to be no related parties of the entity which require reporting during the year (2022: none).

These unaudited financial statements have been subjected to independent examination. See report on page 8.

PSI-K

England & Wales - Charity number 1126308

Accounts

Company registration number 06440198

PSI-K

(A company limited by guarantee)

REPORT AND UNAUDITED FINANCIAL STATEMENTS

YEAR ENDED 31 DECEMBER 2022

PSI-K
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YEAR ENDED 31 DECEMBER 2022

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**PSI-K
LEGAL AND ADMINISTRATIVE INFORMATION
YEAR ENDED 31 DECEMBER 2022**

Psi-k is a company limited by guarantee and a registered charity governed by its Memorandum and Articles of Association dated 29 November 2007.

Company registration number: 06440198

Charity registration number: 1126308

DIRECTORS AND TRUSTEES

The directors of the company are its Trustees for the purpose of Charity Law and throughout this report are collectively referred to as the Trustees. The Trustees who served during the period and to the date of this report are set on page 4.

SECRETARY

Damian Jones

REGISTERED AND PRINCIPAL OFFICE

Stfc Scitech Daresbury
Daresbury
Warrington
Cheshire
WA4 4AD

ACCOUNTANTS & INDEPENDENT EXAMINERS

RSM UK Tax and Accounting Limited
Chartered Accountants
5th Floor
One City Place
Queens Road
Chester
CH1 3BQ

BANKERS

HSBC Bank Plc
11 Stamford New Road
Altrincham
Cheshire
WA14 1BW

**PSI-K
REPORT OF THE CHAIRMAN
YEAR ENDED 31 DECEMBER 2022**

2022 was a resurgent year for Psi-k with the twice-postponed Psi-k Conference proving to be an outstanding success. This was the sixth general conference for the worldwide Psi-k community, following previous successful events held in San Sebastian (2015), Berlin (2010), and Schwäbisch Gmünd (2005, 2000, 1996). The 2022 Conference was a fully in-person event held over 3.5 days (22–25 August) at the SwissTech Convention Centre at the École Polytechnique Fédérale de Lausanne (EPFL) in Switzerland. It attracted 1,269 registered participants, exceeding all expectations, as the opportunity for the community to gather in person after a two-year hiatus caused by the Covid-19 pandemic proved to be extremely attractive. The participants included 461 PhD students, 301 postdocs and 374 established academics or senior researchers along with 40 from industry. 21.5% of participants were female. Over 80% of the participants were based at institutions in Europe, owing to the travel restrictions still in place at the time. The scientific programme included six plenary lectures, 38 symposia (with 372 talks) and 715 posters.

The plenary lectures were delivered by Lucia Reining, Nicola Spaldin, Feliciano Giustino, Francesco Mauri, Angelos Michaelides and Gábor Csányi. Overall poster prizes were awarded to Jennifer Coulter (Harvard), Chengcheng Xiao (Imperial College London), Niamh O'Neill (Cambridge) and Divya Suman (EPFL). An important addition to the programme for 2022 was a session organised by and for early career researchers, whose involvement in Psi-k is crucial for its future – this was led by Joseph Prentice (Oxford), Michele Kotiuga (EPFL) and Valerio Vitale (Trieste). A gala social event was held on the evening of 24 August in the centre of Lausanne. A comprehensive survey was sent to all participants and the responses were overwhelmingly positive – further details can be found at the Conference web site: <https://www.psik2022.net>. Psi-k gratefully acknowledges the support from its sponsors for this event but especial thanks are due to Nicola Marzari, Conference Chair, and Patrick Mayor, Principal Organiser, for their hard work and dedication to ensuring the success of the Conference both scientifically and practically.

In addition to the Conference, Psi-k sponsored a further 19 workshops, summer schools and hands-on tutorials, details of which can be found at <https://psi-k.net/psi-k-workshops-2022/>.

One Psi-k highlight was published in March on “Non-linear response of solids and nanostructures: a real-time prospective” by Claudio Attacalite, Davide Sangalli and Myrta Grüning. This can be found at <https://psi-k.net/highlights/>, together with all those published from 1994 onwards. We are always keen and happy to showcase work that combines breadth and depth and is relevant to the Psi-k community; any suggested contributions can be discussed with leon.petit@stfc.ac.uk. We have established informal agreements with npj Computational Materials and IOP Electronic Structure that provide opportunities for the open-access publication of approved Psi-k highlights.

All these activities are supported by the generous donations of groups worldwide – 38 groups or institutions from 12 countries contributed to the charity in 2022. Anyone (individuals, groups, organisations, companies) who would like to contribute can contact p.haynes@imperial.ac.uk and PSIK_ADMIN@stfc.ac.uk.

The Working Groups were last reorganised in 2017, and remain instrumental in coordinating the scientific programme. The 16 Working Groups are organised by three main themes, each overseen by a Trustee:

- A. Physical formalisms – Silke Biermann (École Polytechnique, Paris)
- B. Algorithms, software and data – Arash Mostofi (Imperial College London)
- C. Applications to real materials and materials design – Igor Abrikosov (Linköpings Universitet)

Further information about the Working Groups can be found at <https://psi-k.net/groups/>. At the Conference it was announced that a further review of the Working Groups would take place, and a meeting of Trustees and current Working Group Leaders was held after the end of the Conference to discuss the feedback from the community.

**PSI-K
REPORT OF THE CHAIRMAN (Continued)
YEAR ENDED 31 DECEMBER 2022**

In 2022 the two-step submission process for workshop proposals continued, whereby a first deadline at the end of July is used for outline proposals, which are light-touch submissions to be evaluated by the Working Groups and Trustees in order to coordinate and streamline all activities. Outline proposals are either encouraged to submit a full proposal by the end of October, rejected right away, or advised to merge with other efforts on similar themes to avoid duplication. The Psi-k/CECAM Research Conference has a separate application track, and any proposals not selected but deemed of sufficient quality can directly apply as a full proposal: partly as a result of the Conference there was no Psi-k/CECAM Research Conference in 2022.

The Board of Trustees met five times in 2021, all by teleconference: on 17 February, 21 April, 23 June, 15 September and 1 November. Minutes of meetings are recorded, circulated, and kept for internal use. The Trustees (<https://psi-k.net/admin/>), plus 19 Working Group leaders (<https://psi-k.net/groups/>) and members of the Scientific Advisory Committee (<https://psi-k.net/scientific-advisory-committee/>) attended the Annual Meeting on 25 November, where all activities are finalised for the following year (in this case, from April 2023 to March 2024). The third online community meeting was held on 9 December and advertised to the whole Psi-k mailing list. This included a review of the Conference as well as items about encouraging the involvement of early career researchers and feedback on the Working Groups.

The generous contribution of time from all the groups above is essential to the wellbeing of the Charity, but particular thanks must go to our Operations Manager Damian Jones (STFC Daresbury Laboratory, UK) for coordinating all the administration; and to Risto Nieminen who stepped down as a Trustee at the end of 2022 having been involved from the earliest days of the Network.



Peter Haynes - Psi-K Chair

Date: 20/09/23

**PSI-K
REPORT OF THE TRUSTEES
YEAR ENDED 31 DECEMBER 2022**

The Trustees present their annual report and unaudited financial Statements for the year ended 31 December 2022.

Trustees

The Trustees who served during the period and to the date of this report were:

Igor Abrikosov
Silke Biermann
Stefan Blügel
Claudia Draxl
+Martin Friak
Peter Haynes (Chair)
Nicola Marzari
+Angelos Michaelides
Elisa Molinari
Arash Mostofi
*Risto Nieminen
Lucia Reining

The Trustee whose name is starred (*) resigned following the Annual Meeting on 26 November 2021, and at this same meeting the Trustees whose names are indicated by a plus (+) were elected.

Structure, governance and management

The organisation is governed by its Memorandum and Articles of Association and is a registered company limited by guarantee.

Psi-k is a Europe-based, worldwide network of researchers working on the advancement of first-principles computational materials science. Its mission is to develop fundamental theory, algorithms, and computer codes in order to understand, predict, and design materials properties and functions. Theoretical condensed matter physics, quantum chemistry, thermodynamics, and statistical mechanics form its scientific core. Applications encompass inorganic, organic and bio-materials, and cover a whole range of diverse scientific, engineering, and industrial endeavours. Key activities of Psi-k are the organisation of conferences, workshops, tutorials and training schools as well as the dissemination of scientific thinking in society.

Psi-k has a minimum of three Trustees, but there is no maximum. On the date of this report there were eleven Trustees.

Psi-k has a Chair, and a Scientific Advisory Committee (SAC) of about 80 members, which is headed by the Chair of Psi-k. In addition all Trustees are also SAC members.

The Board of Trustees meets on average five to six times a year, normally with a combination of face-to-face meetings and teleconference meetings. In 2022 there were five meetings, all by teleconference: on 17 February, 21 April, 23 June, 15 September and 1 November. The Trustees had opportunities to meet in person during and after the Psi-k Conference in Lausanne (22–26 August) and at the Annual Meeting 26 November (following the Annual Meeting of the SAC). Minutes of meetings are recorded, circulated, and kept for internal use. The Board of Trustees uses these meetings to discuss matters including but not limited to: future strategy, funding and finances, events such as workshops, conferences and summer schools, and relationships with external organisations such as CECAM.

The day to day running of Psi-k is delegated to the Chair, Peter Haynes, supported by the Operations Manager and Secretary, Damian Jones.

The SAC meets once a year, normally in November, together with the leaders of the 16 Working Group (<https://psi-k.net/groups/>). It is chaired by the Chair of Psi-k and its role is to make recommendations to the Board, particularly regarding plans for all activities for the following year (in this case, from April 2023 to March 2024). In 2022 the Annual Meeting was held on 25 November in hybrid mode: in person in Paris and online.

For the third time, on 9 December 2022, an open community meeting was held online and advertised via the Psi-k mailing list.

These unaudited financial statements have been subjected to independent examination. See report on page 8.

PSI-K
REPORT OF THE TRUSTEES (Continued)
YEAR ENDED 31 DECEMBER 2022

All Trustees gave their time freely and no Trustee remuneration was paid in the year: expenses paid to Trustees amounted to €nil. Trustees are required to disclose all relevant interests and register them with the Chair.

Trustees are required to declare any conflicts of interest at each meeting and these are recorded in the minutes. If a vote of the Trustees is required on a matter, a Trustee who has declared a conflict of interest on that matter may not cast a vote.

Risk management

The Trustees have considered the major risks to which the charity is exposed and have reviewed those risks and established systems and procedures to manage those risks.

A significant risk for the Psi-k Charity is reduced financial funding. Since 2016, Psi-k has been sustained entirely by donations. In 2021 the Trustees agreed that our annual expenditure on community activities is determined by our income from the previous year, and adopted a target for reserves of €200,000.

Objectives and activities

Europe has become the leading research area in the world for the application of first-principles computational modelling to materials science and Psi-k aims to maintain and enhance this status.

“Psi-k research” covers structures, properties and processes in all types of materials at the atomic level and in nanometre-scale structures, studied by ab initio quantum-mechanical computer simulation. A series of working groups represent the views of the community and organise activities to deliver the Psi-k mission. In 2022 these were:

Theme A: Physical Formalisms	
WG A1	Density and density-matrix functional theories
WG A2	Perturbative many-body methods
WG A3	Non-perturbative many-body methods
WG A4	Open and non-equilibrium systems
WG A5	Quasi-particle interactions and spectroscopies
Theme B: Algorithms, Software and Data	
WG B1	Reduced-scaling methods
WG B2	Statistics and configuration sampling
WG B3	Bridging length- and time-scales
WG B4	Software engineering
WG B5	High-throughput screening and data analytics
Theme C: Applications to Real Materials and Materials Design	
WG C1	Structural materials
WG C2	Functional materials and devices
WG C3	Magnetism and spintronics
WG C4	Surfaces and interfaces
WG C5	Nanoscale structures (2D, 1D, 0D) and related phenomena
WG C6	Molecules, macromolecules and biomolecules

Psi-k will promote and coordinate collaboration within the European research community by, among others, the following measures:

- supporting workshops and small conferences on specific topics of active research;
- supporting summer schools, tutorial courses and other training activities for young and new researchers in the field;
- organising a large “Psi-k conference” (such as those previously held in 1996, 2000, 2005, 2010 and 2015) every five years, this was the highlight of the year, held 22–25 August 2022 at EPFL in Switzerland;
- disseminating information about research progress, job opportunities, relevant workshops, conferences and other events, and funding opportunities via the Psi-k website providing a portal and a newsletter available freely to anyone in the world by electronic means.

**PSI-K
REPORT OF THE TRUSTEES (Continued)
YEAR ENDED 31 DECEMBER 2022**

The activities are open to all researchers in the field. Psi-k acts as a vehicle to engaging with the wider scientific community, with industry, European policy makers and trans-European computer centres. It will seek to maintain cooperation with organisations such as the Centre Européen de Calcul Atomique et Moléculaire (CECAM), the European molecular simulation community and its networks and Psi-k's counterpart research communities on other continents.

Aims and objectives for 2022

The highlight of 2022 was the twice-postponed Psi-k Conference, held fully in person at EPFL in Lausanne in August. This was the largest in-person conference held since the pandemic and was extremely successful: further details are provided in the Chair's report. The other main activities planned during 2022 comprised the scientific programme of workshops, tutorials and summer schools on the electronic structure of complex processes in materials, i.e. the topic of the Psi-k Charity. In view of the Psi-k Conference, no Psi-k/CECAM Research Conference was held in 2022 and no events were funded in the period around the Conference. The programme comprised 20 events in 2022, including the Conference.

Grant making policy

The Psi-k Charity does not make grants to other research bodies.

The Psi-k Charity applies its funding to the organization of workshops, summer schools, hands-on courses and the Psi-k Conference. The Theoretical and Computational Physics Group at STFC Daresbury Laboratory publishes the Psi-k Newsletter and provides administrative support.

The achievements of every workshop to which Psi-k contributes are monitored in the form of a report which is published on the Psi-k website (<http://psi-k.net/>).

Key performance indicators

In 2022 the Psi-k Charity organised 20 workshops, conferences and training activities. This is less than a normal year but accounted for by the priority given to the large in-person Psi-k Conference.

Financial review 2022 and plan for 2023

Member donations in 2022 were slightly up from the previous year with a total of about €123,600 received. The expenses in the 2022 budget included €87,342 for workshops, and €15,000 for the Psi-k Conference leading to total expenses of about €102,342.

At the year end the net assets comprise the bank balances of €433,267 (2021: €471,443) and debtors of €150,583 (2021: €35,825), which have increased significantly at the year end, in the main due to a €100,000 return of capital contribution post year end, due to the popularity of a seminar held during the year which meant the contribution to costs was not required by PSI-K. Liabilities include grant creditors & accruals of €168,919 (2021: €168,313).

Plan for 2023: The Trustees continue to seek new contributors with an aim of increasing annual donations to around €150,000. The amount of €102,745 will be spent on workshops in the coming 2023 seminar season. Any deficit will be covered by the reserves.

During the year 2022 the Trustees were satisfied that, as far as circumstances permitted, the Charity continued to benefit the public through its activities targeted to achieve its charitable objectives.

Public Benefit

The Trustees confirm that they have referred to the guidance contained in the Charity Commission's general guidance on public benefit when reviewing the Trust's aims and objectives and in planning future activities and setting the grant making policy for the year.

Trustees' responsibilities

The Trustees (who are also Directors of Psi-k for the purposes of company law) are responsible for preparing the Trustees' Annual Report and the financial statements in accordance with applicable law and United Kingdom Accounting Standards (United Kingdom Generally Accepted Accounting Practice).

Company Law requires the Trustees to prepare financial statements for each financial year which give a true and fair view of the state of affairs of the charitable company and of the incoming resources and applications of resources, including the income and expenditure, of the charitable company for that year.

These unaudited financial statements have been subjected to independent examination. See report on page 8.

PSI-K
REPORT OF THE TRUSTEES (Continued)
YEAR ENDED 31 DECEMBER 2022

In preparing those financial statements, the Trustees are required to:

- provide statements on the going concern basis unless it is inappropriate to presume that the charitable company will continue in business;
- select suitable accounting policies and apply them consistently;
- observe the methods and principles in the Charitable SORP
- make judgements and estimates that are reasonable and prudent;
- state whether applicable accounting standards have been followed, subject to any material departures disclosed and explained in the financial statements.

The Trustees are responsible for keeping proper accounting records that disclose with reasonable accuracy at any time the financial position of the charitable company and enable them to ensure that the financial statements comply with the Companies Act 2006. They are also responsible for safeguarding the assets of the charitable company and hence for taking reasonable steps for the prevention of fraud and other irregularities.

This report has been prepared in accordance with the Statement of Recommended Practice: Accounting and Reporting by Charities (issued in March 2005) and in accordance with the special provisions applicable to small companies under part 15 of the Companies Act 2006.

ON BEHALF OF THE BOARD



Peter Haynes

Date: 20/09/23

INDEPENDENT EXAMINER'S REPORT TO THE TRUSTEES OF PSI-K

I report to the trustees on my examination of the financial statements of PSI-K ("the company") for the year ended 31 December 2022, which are set out on pages 9 to 16.

Responsibilities and basis of report

As the trustees of the company (and also its directors for the purposes of company law) you are responsible for the preparation of the financial statements in accordance with the requirements of the Companies Act 2006 ('the 2006 Act').

Having satisfied myself that the financial statements of the company are not required to be audited under Part 16 of the 2006 Act and are eligible for independent examination I report in respect of my examination of your charity's financial statements as carried out under section 145 of the Charities Act 2011 ('the 2011 Act'). In carrying out my examination I have followed the Directions given by the Charity Commission under section 145 (5)(b) of the 2011 Act.

An independent examination does not involve gathering all the evidence that would be required in an audit and consequently does not cover all the matters that an auditor considers in giving their opinion on the financial statements. The planning and conduct of an audit goes beyond the limited assurance that an independent examination can provide. Consequently, I express no opinion as to whether the financial statements present a 'true and fair view' and my report is limited to those specific matters set out in the independent examiner's statement.

Independent examiner's statement

I have completed my examination. I confirm that no material matters have come to my attention in connection with the examination giving me reasonable cause to believe that in any material respect:

1. accounting records were not kept in respect of the company as required by section 386 of the 2006 Act; or
2. the financial statements do not accord with those records; or
3. the financial statements do not comply with the accounting requirements of section 396 of the 2006 Act other than any requirement that the financial statements give a 'true and fair view' which is not a matter considered as part of an independent examination; or
4. the financial statements have not been prepared in accordance with the methods and principles of the Statement of Recommended Practice: Accounting and Reporting by Charities applicable to charities preparing their financial statements in accordance with the Financial Reporting Standard applicable in the UK and Ireland (FRS 102).

I have no concerns and have come across no other matters in connection with the examination to which attention should be drawn in this report in order to enable a proper understanding of the financial statements to be reached.

John Guest

Name: **John Guest**

Name of applicable listed body: **The Institute of Chartered Accountants in England and Wales**

Relevant professional qualification or membership of professional body: **Chartered Accountant**

ON BEHALF OF RSM UK TAX AND ACCOUNTING LIMITED

Chartered Accountants

5th Floor

One City Place

Queens Road

Chester

CH1 3BQ

Date: 20/09/23

PSI-K
STATEMENT OF FINANCIAL ACTIVITIES
INCLUDING INCOME AND EXPENDITURE ACCOUNT
YEAR ENDED 31 DECEMBER 2022

	Notes	Unrestricted Funds €	Total Funds 2022 €	Total Funds 2021 €
INCOMING RESOURCES				
Donations and legacies				
- Donated services		37,364	37,364	37,364
Charitable activities				
- Donations from research bodies		101,499	101,499	170,257
TOTAL INCOMING RESOURCES		<u>138,863</u>	<u>138,863</u>	<u>207,621</u>
RESOURCES EXPENDED				
Charitable activities	4	62,887	62,887	54,223
TOTAL RESOURCES EXPENDED		<u>62,887</u>	<u>62,887</u>	<u>54,223</u>
NET INCOMING RESOURCES AND NET MOVEMENT IN FUNDS FOR THE YEAR		<u>75,976</u>	<u>75,976</u>	<u>153,398</u>
RECONCILIATION OF FUNDS				
TOTAL FUNDS BROUGHT FORWARD		<u>338,955</u>	<u>338,955</u>	<u>185,557</u>
TOTAL FUNDS CARRIED FORWARD	12	<u><u>414,931</u></u>	<u><u>414,931</u></u>	<u><u>338,955</u></u>

The statement of financial activities includes all gains and losses recognised in the year.

All income and expenditure derive from continuing activities and are attributed to unrestricted funds.

The statement of financial activities also complies with the requirements for an income and expenditure account under the Companies Act 2006.

**PSI-K
BALANCE SHEET
AS AT 31 DECEMBER 2022**

Company registration number 06440198

	Notes	2022 €	2021 €
CURRENT ASSETS			
Debtors	9	150,583	35,825
Cash at bank		433,267	471,443
		<u>583,850</u>	<u>507,268</u>
CREDITORS: Amounts falling due within one year	10	(168,919)	(168,313)
		<u></u>	<u></u>
TOTAL ASSETS LESS CURRENT LIABILITIES		<u>414,931</u>	<u>338,955</u>
INCOME FUNDS			
Unrestricted funds	12	414,931	338,955
Restricted funds	12	-	-
		<u></u>	<u></u>
TOTAL CHARITY FUNDS	12	<u>414,931</u>	<u>338,955</u>

For the year ending 31 December 2022 the company was entitled to exemption from audit under Section 477 of the Companies Act 2006 relating to small companies.

The members have not required the company to obtain an audit of its financial statements for the year ended 31 December 2022 in accordance with Section 476 of the Companies Act 2006.

The directors acknowledge their responsibilities for:

- ensuring that the company keeps accounting records which comply with Section 396 of the Companies Act 2006; and
- preparing financial statements which give a true and fair view of the state of affairs of the company as at the end of each financial year and of its profit or loss for each financial year in accordance with the requirements of Section 396 and which otherwise comply with the requirements of the Companies Act 2006 relating to financial statements, so far as applicable to the company.

These financial statements are prepared in accordance with the provisions applicable to companies subject to the small companies regime and in accordance with Charities SORP (FRS102).

The notes on pages 11 to 17 form part of these financial statements.

The financial statements were approved by the Trustees and authorised for issue on 20/09/23..... and were signed on their behalf by:



Peter Haynes (Chair)

Trustee

These unaudited financial statements have been subjected to independent examination. See report on page 8.

PSI-K
NOTES TO THE FINANCIAL STATEMENTS
YEAR ENDED 31 DECEMBER 2022

1. ACCOUNTING POLICIES

a. Basis of preparation

The financial statements have been prepared in accordance with Accounting and Reporting by Charities: Statement of Recommended Practice applicable to charities preparing their financial statements in accordance with the Financial Reporting Standard applicable in the UK and Republic of Ireland (FRS 102) (Issued October 2019) - (Charities SORP (FRS 102)), the Financial Reporting Standard applicable in the UK and Republic of Ireland (FRS 102) and the Companies Act 2006.

The financial statements are prepared in Euro and amounts in these financial statements are rounded to the nearest Euro.

PSI-K meets the definition of a public benefit entity under FRS 102. Assets and liabilities are initially recognised at historical cost or transaction value unless otherwise stated in the relevant accounting policy notes. The Charity has taken advantage of the provisions in the SORP for Charities applying FRS102 Update Bulletin 1 not to prepare a Statement of Cash Flows.

b. Preparation of the financial statements on a going concern basis

The trustees forecast that the charity will continue to be able to pay its liabilities as they fall due for a period of at least 12 months following the date of approving the financial statements. The forecasts take into account transactions that are anticipated to take place in the foreseeable future and indicate that no additional financial resources will be required should the actual performance differ from forecast. On this basis the trustees have concluded that adopting the going concern basis of accounting in preparing the annual financial statements is appropriate.

c. Income recognition

Incoming resources represents donations from research bodies in Europe to support the company's activities, less amounts carried forward to future periods as deferred income; and donated services, which are included based on the hours worked and the appropriate hourly rate. Income is recognised when the entity has entitlement to the funds, it is probable that the income will be received and the amount can be measured reliably.

d. Donated services

Donated services are included within incoming resources with an equivalent amount shown within resources expended, where the benefit to the charity is reasonably quantifiable, measurable and material. The value placed on these resources is the estimated value to the charity of the service received.

e. Deferred income

Donations received in advance of the period that they relate to, or which are provided specifically for future periods, are carried forward as deferred income. These amounts relate to contributions from research bodies received in advance.

f. Expenditure recognition

All expenditure is accounted for on an accruals basis, inclusive of any VAT which cannot be recovered.

Grants payable are payments made to third parties in the furtherance of the charitable objectives of the Charity. Grants are accounted for when either the recipient has a reasonable expectation that they will receive a grant and the trustees have agreed to pay the grant without condition, or the recipient has a reasonable expectation that they will receive a grant and any condition attaching to the grant is outside of the control of the Charity.

Provisions for grants are made when the intention to make a grant has been communicated to the recipient but there is uncertainty about either the timing of the grant or the amount of grant payable.

Governance costs are related to the governance of the charity, such as the costs of preparing the financial statements and statutory compliance.

Irrecoverable VAT is charged as a cost against the activity for which the expenditure was incurred.

These unaudited financial statements have been subjected to independent examination. See report on page 8.

PSI-K
NOTES TO THE FINANCIAL STATEMENTS
YEAR ENDED 31 DECEMBER 2022

1. ACCOUNTING POLICIES (Continued)

g. Charitable Funds

Restricted funds are to be used for specified purposes as laid down by the donor. Expenditure which meets these criteria is identified to the fund, together with a fair allocation of management and support costs.

Unrestricted funds are available for use at the discretion of the Trustees in furtherance of the general objectives of the Charity.

h. Foreign currencies

The trustees consider that the functional currency of the charity is the Euro, as most transactions are denominated and are carried out in that currency.

Assets and liabilities denominated in other currencies are translated into Euros at the rate of exchange ruling at the balance sheet date. Transactions in other currencies are translated into Euros at the rate of exchange ruling at the date of the transaction. Exchange differences are taken into account in arriving at the net movement in funds in the Statement of Financial Activities.

At the balance sheet date the rate of exchange between Sterling and Euro was £1 equals €1.1295 (2021: €1.1893).

i. Financial instruments

The Charity has elected to apply the provisions of Section 11 'Basic Financial Instruments' and Section 12 'Other Financial Instruments Issues' of FRS 102, in full, to all of its financial instruments.

Financial assets and financial liabilities are recognised when the Charity becomes a party to the contractual provisions of the instrument, and are offset only when the Charity currently has a legally enforceable right to set off the recognised amounts and intends either to settle on a net basis, or to realise the asset and settle the liability simultaneously.

j. Basic Financial assets

Trade and other debtors (including accrued income) which are receivable within one year and which do not constitute a financing transaction are initially measured at the transaction price and subsequently measured at amortised cost, being the transaction price less any amounts settled and any impairment losses.

k. Basic Financial liabilities

Financial instruments are classified as liabilities according to the substance of the contractual arrangements entered into.

Trade and other creditors (including accruals) payable within one year that do not constitute a financing transaction are initially measured at the transaction price and subsequently measured at amortised cost, being the transaction price less any amounts settled.

l. Derecognition of financial liabilities

Financial liabilities are derecognised when the charity's contractual obligations expire or are discharged or cancelled

2. CRITICAL ACCOUNTING ESTIMATES AND JUDGMENT

In the application of the Charity's accounting policies, the trustees are required to make judgements, estimates and assumptions about the carrying amount of assets and liabilities that are not readily apparent from other sources. The estimates and associated assumptions are based on historical experience and other factors that are considered to be relevant. Actual results may differ from these estimates.

The estimates and underlying assumptions are reviewed on an on-going basis. Revisions to accounting estimates are recognised in the period in which the estimate is revised where the revision affects only that period, or in the period of the revision and future periods where the revision affects both current and future periods.

No critical accounting estimates and judgements have been made in preparing these financial statements.

These unaudited financial statements have been subjected to independent examination. See report on page 8.

PSI-K
NOTES TO THE FINANCIAL STATEMENTS
YEAR ENDED 31 DECEMBER 2022

3. INCOME

Donations received from research bodies attributable to overseas markets total 96% (2021: 97%). All income received in 2022 (and 2021) was unrestricted.

4. TOTAL EXPENDITURE

	Grant Funding of Activities €	Support Costs €	Total 2022 €	Total 2021 €
Charitable Activities				
Grants payable	5,860	-	5,860	8,077
Support costs	-	41,886	41,886	38,223
Prize giving awards and donations	-	6,500	6,500	2,000
Exchange losses / (gains)	-	517	517	(1,189)
Governance Costs (Note 5)	-	8,124	8,124	7,112
	<u>5,860</u>	<u>57,027</u>	<u>62,887</u>	<u>54,223</u>

Total expenditure for the year was €62,887, all of which was unrestricted expenditure (2021: €54,223).

The grant funding of activities totalling €5,860 (2021: €8,077) relates to payments made to institutions regarding scientific conferences.

	2022 €	2021 €
Support costs comprise:		
Bank charges	521	621
Donated services	37,364	37,364
Other support costs	4,001	238
	<u>41,886</u>	<u>38,223</u>

It is estimated that the charity benefited from approximately 636 (2021: 636) hours of donated time provided to assist with the running of the charity. This figure was made up of 477 (2021: 477) hours of donated time received as a contribution in kind from the CCP9 service level agreement, and 159 (2021: 159) hours from the Science and Technology Facilities Council.

5. GOVERNANCE COSTS

	Total 2022 €	Total 2021 €
Governance costs are made up of the following:		
Independent examiners fee	3,863	3,926
Accountancy	4,261	2,048
Corporation tax	-	1,138
	<u>8,124</u>	<u>7,112</u>

6. STAFF COSTS

There were no employees in the year. No employees received employee benefits over €70,000.

The Trustees were not paid any remuneration and so there is no remuneration paid to key management personnel. No expenses were incurred or reimbursed during the year (2021: Nil).

These unaudited financial statements have been subjected to independent examination. See report on page 8.

PSI-K
NOTES TO THE FINANCIAL STATEMENTS
YEAR ENDED 31 DECEMBER 2022

7. TAXATION

PSI-K is a registered charity and is therefore exempt from tax on its charitable income.

8. GRANTS MADE TO INSTITUTIONS	2022	2021
	€	€
Grants awarded in the year were all to institutions and comprised:		
CECAM, Lausanne	13,500	4,000
EPFL, Switzerland	-	3,600
Aarhus Institute of Advanced Studies (AIAS), Denmark	-	4,310
The Abdus Salam International Centre for Theoretical Physics, Italy	-	10,000
Aachen, Germany	-	3,000
Guidel, France	-	4,500
ICTP Trieste (Italy)	16,500	5,000
Daresbury Laboratory, UK	-	4,860
Stockholm University, Stockholm, Sweden	-	9,000
Leuven, Belgium	-	12,000
Bordeaux, France	-	3,600
Erice (Italy)	-	4,000
University of Warwick UK	-	3,600
Gran Sasso Science Institute, L'Aquila, Italy	-	8,400
Ekaterinburg, Russia	-	7,875
Benasque Center for Science (Benasque, Spain)	-	12,000
Castle Reisenburg near Gunzburg/Germany	-	3,000
Alto University, Helsinki, Finland	12,050	-
STFC Rutherford Appleton Laboratory, UK	4,000	-
Forschungszentrum Julich, Germany	2,500	-
Rome, Italy	3,750	-
Ecole Normale Supérieure, Paris, France	6,000	-
CECAM-ISR, Tel Aviv University, Israel	4,000	-
Zaragoza, Spain	6,000	-
Berlin, Germany	20,000	-
Modena	4,500	-
Bangalore, India	5,000	-
Orebro, Sweden	5,000	-
University of Pavia, Italy	5,000	-
Athens, Greece	4,000	-
Albert-Ludwigs-Universität Freiburg, Germany	3,600	-
London, UK	3,000	-
National Graphene Institute, Manchester UK	3,000	-
Paphos, Cyprus	5,000	-
Reingberg, Tegernsee, Germany	5,000	-
Les Houches School of Physics, France	6,000	-
Total institutional grants	137,400	102,745
Reconciliation of grants payable		
Grant commitments brought forward	154,034	177,516
Commitments made during the year	137,400	102,745
Physics by the lake additional 2018 grant	-	1,000
Grant commitments for the year	137,400	103,745
Grants cancelled, recovered or refunded	(131,540)	(95,668)
Grants payable for the year (note 4)	5,860	8,077
Grants paid during the year	(98,904)	(48,359)
Grants to be refunded post year end transferred to other debtors (note 9)	100,000	12,800
Grants refunded in the year	-	4,000
Grant commitments carried forward	160,990	154,034

These unaudited financial statements have been subjected to independent examination. See report on page 8.

PSI-K
NOTES TO THE FINANCIAL STATEMENTS
YEAR ENDED 31 DECEMBER 2022

9. DEBTORS	2022 €	2021 €
Trade debtors	40,583	23,025
Accrued income	10,000	-
Other debtors	100,000	12,800
	<u>150,583</u>	<u>35,825</u>
	<u><u>150,583</u></u>	<u><u>35,825</u></u>
10. CREDITORS: Amounts falling due within one year	2022 €	2021 €
Grant commitments	160,990	154,034
Accruals	7,929	7,279
Deferred income (note 11)	-	7,000
	<u>168,919</u>	<u>168,313</u>
	<u><u>168,919</u></u>	<u><u>168,313</u></u>
11. DEFERRED INCOME	2022 €	2021 €
Deferred income as at 1 January	7,000	6,000
Received in year	-	7,000
Released in year	(7,000)	(6,000)
	<u>-</u>	<u>7,000</u>
Deferred income as at 31 December	<u><u>-</u></u>	<u><u>7,000</u></u>

Deferred income comprises contributions from research bodies received pre 31 December 2022 which have been invoiced in advance.

12. STATEMENT OF FUNDS

The movements on the funds of the charity were as follows:

	Balance 01.01.22 €	Income €	Expenditure €	Transfer €	Balance 31.12.22 €
Unrestricted Funds					
General Fund	338,955	138,863	(62,887)	-	414,931
	<u>338,955</u>	<u>138,863</u>	<u>(62,887)</u>	<u>-</u>	<u>414,931</u>
	<u><u>338,955</u></u>	<u><u>138,863</u></u>	<u><u>(62,887)</u></u>	<u><u>-</u></u>	<u><u>414,931</u></u>
Total Funds	<u><u>338,955</u></u>	<u><u>138,863</u></u>	<u><u>(62,887)</u></u>	<u><u>-</u></u>	<u><u>414,931</u></u>

These unaudited financial statements have been subjected to independent examination. See report on page 8.

PSI-K
NOTES TO THE FINANCIAL STATEMENTS
YEAR ENDED 31 DECEMBER 2022

12. STATEMENT OF FUNDS (continued)

The movement on the funds of the charity in 2021 were as follows:

	Balance 01.01.21	Income	Expenditure	Transfer	Balance 31.12.21
	€	€	€	€	€
Unrestricted Funds					
General Fund	185,557	207,621	(54,223)	-	338,955
	<u>185,557</u>	<u>207,621</u>	<u>(54,223)</u>	<u>-</u>	<u>338,955</u>
Total Funds	<u>185,557</u>	<u>207,621</u>	<u>(54,223)</u>	<u>-</u>	<u>338,955</u>

All funds for the year ended 31 December 2022 and year ended 31 December 2021 relate to unrestricted reserves.

13. ANALYSIS OF NET ASSETS BETWEEN FUNDS

	Unrestricted Funds €	Total 2022 €
Fund balances at 31 December 2022 are represented by:		
Current assets	583,850	583,850
Creditors: Amounts falling due within one year	(168,919)	(168,919)
Total Net Assets	<u>414,931</u>	<u>414,931</u>
	Unrestricted Funds €	Total 2021 €
Fund balances at 31 December 2021 are represented by:		
Current assets	507,268	507,268
Creditors: Amounts falling due within one year	(168,313)	(168,313)
Total Net Assets	<u>338,955</u>	<u>338,955</u>

14. GUARANTEE COMPANY AND LIABILITY OF MEMBERS

Psi-k is a company limited by guarantee and therefore does not have any share capital.

The liability of members is limited. In the event of the charity being wound up during a member's period of membership or within one year after ceasing to be a member, an amount not exceeding the sum of £1 may be required from that member towards the payment of the debts and liabilities of the company incurred before membership ceased and the costs of winding up.

At 31 December 2022, the company had 10 (2021: 10) members.

15. RELATED PARTY

There are deemed to be no related parties of the entity which require reporting during the year.

PSI-K

England & Wales - Charity number 1126308

Accounts

Charity Registration No. 1126308

Company Registration No. 06440198 (England and Wales)

PSI-K

(A COMPANY LIMITED BY GUARANTEE)

**REPORT AND UNAUDITED FINANCIAL
STATEMENTS
FOR THE YEAR ENDED
31 DECEMBER 2021**

PSI-K
(A COMPANY LIMITED BY GUARANTEE)
LEGAL AND ADMINISTRATIVE INFORMATION

Trustees	Igor Abrikosov Silke Biermann Stefan Blugel Claudia Draxl Nicola Marzari Elisa Molinari Arash Mostofi Risto Nieminen Lucia Reining Peter Haynes (Chair Person)
Secretary	D Jones
Charity number	1126308
Company number	06440198
Registered office	Stfc Scitech Daresbury Daresbury Warrington WA4 4AD
Independent examiner	RSM UK Tax and Accounting Limited Chartered Accountants 5th Floor One City Place Queens Road Chester CH1 3BQ
Bankers	HSBC Bank Plc 11 Stamford New Road Altrincham Cheshire WA14 1BW

PSI-K (A COMPANY LIMITED BY GUARANTEE) TRUSTEES' REPORT (INCLUDING DIRECTORS' REPORT) FOR THE YEAR ENDED 31 DECEMBER 2021

Chair's Report

2021 was another challenging year for Psi-k that has traditionally relied heavily on face-to-face interactions for its activities. However members of our community demonstrated their ingenuity in adapting to the rapidly changing circumstances and accompanying restrictions. Out of over 30 workshops, summer schools and hands-on tutorials that were originally planned to take place in 2021, just under half were held fully online, the highlight among these being the Psi-k/CECAM Research Conference on "New horizons in nucleation: a playground for classical and ab initio simulation methods" that was postponed from 2020. As the Covid situation improved in the summer and autumn, three events were held in hybrid mode (both in person and online) and seven took place fully in person. Only three activities were postponed to 2022 and three were cancelled.

As reported last year, the major quinquennial Psi-k Conference had been planned to take place in Lausanne in September 2020 but this has been postponed until August 2022, and registrations for a fully in-person conference are expected to open in March 2022. Originally the Volker Heine Young Investigator Award had been planned to occupy a symposium at the Conference, but in order to avoid too long a gap between awards, this was held online on 9 September 2021. Five finalists were selected and delivered presentations, with Dr Bingqing Cheng, now Assistant Professor at the Institute of Science and Technology Austria, selected as the overall winner for her work on "Predicting material properties with the help of machine learning."

Three Psi-k highlights were published in April, June and November, which can be found at <https://psi-k.net/highlights/>, together with all those published from 1994 onwards. We are always keen and happy to showcase work that combines breadth and depth and is relevant to the Psi-k community; any suggested contributions can be discussed with leon.petit@stfc.ac.uk. We have established informal agreements with *npj Computational Materials* and *IOP Electronic Structure* that provide opportunities for the open-access publication of approved Psi-k highlights.

All these activities are supported by the generous donations of groups worldwide – 38 groups or institutions from 12 countries contributed to the charity in 2021. Anyone (individuals, groups, organisations, companies) who would like to contribute can contact p.haynes@imperial.ac.uk and PSIK_ADMIN@stfc.ac.uk.

The Working Groups were reorganised in 2017, and remain instrumental in coordinating the scientific programme. The 16 Working Groups are organised by three main themes, each overseen by a Trustee:

- A. Physical formalisms – Silke Biermann (École Polytechnique, Paris)
- B. Algorithms, software and data – Arash Mostofi (Imperial College London)
- C. Applications to real materials and materials design – Igor Abrikosov (Linköpings Universitet)

Further information about the Working Groups can be found at <https://psi-k.net/groups/>.

In 2021 the two-step submission process for workshop proposals continued, whereby a first deadline at the end of July is used for outline proposals, which are light-touch submissions to be evaluated by the Working Groups and Trustees in order to coordinate and streamline all activities. Outline proposals are either encouraged to submit a full proposal by the end of October, rejected right away, or advised to merge with other efforts on similar themes to avoid duplication. The Psi-k/CECAM Research Conference has a separate application track, and any proposals not selected but deemed of sufficient quality can directly apply as a full proposal: partly as a result of the quinquennial Conference there will not be a Psi-k/CECAM Research Conference in 2022.

The Board of Trustees met six times in 2021, all by teleconference: on 4 February, 22 April, 24 June, 16 September, 21 October and 26 November. Minutes of meetings are recorded, circulated, and kept for internal use. The Trustees (<https://psi-k.net/admin/>), Working Group leaders (<https://psi-k.net/groups/>) and 19 members of the Scientific Advisory Committee (<https://psi-k.net/scientific-advisory-committee/>) attended the Annual Meeting on 26 November, where all activities are finalised for the following year (in this case, from April 2022 to March 2023). Following the success of the first event in 2020, an online community meeting was held before the Annual Meeting and advertised to the whole Psi-k mailing list. The Chair, Peter Haynes, gave an update about Psi-k, and the Conference Chair, Nicola Marzari, provided an updated of plans for the quinquennial Conference. This was followed by a brief time for questions.

PSI-K
(A COMPANY LIMITED BY GUARANTEE)
TRUSTEES' REPORT (CONTINUED)(INCLUDING DIRECTORS' REPORT)
FOR THE YEAR ENDED 31 DECEMBER 2021

The generous contribution of time from all the groups above is essential to the wellbeing of the Charity, but particular thanks must go to our Operations Manager Damian Jones (STFC Daresbury Laboratory, UK) for coordinating all the administration; and to Mike Payne, Angel Rubio and Matthias Scheffler who stepped down as Trustees at the end of 2021 after a combined total of more than 30 years' service.

Trustees' Report

The Trustees present their annual report and unaudited financial statements for the year ended 31 December 2021.

The directors of the company are its Trustees for the purpose of Charity Law and throughout this report are collectively referred to as the Trustees.

Trustees

The Trustees who served during the period and to the date of this report were:

Igor Abrikosov
Silke Biermann
Stefan Blugel
Claudia Draxl
Peter Haynes (Chair)
Nicola Marzari
Elisa Molinari
Arash Mostofi
Risto Nieminen
Mike Payne (resigned 26 November 2021)
Lucia Reining
Angel Rubio (resigned 26 November 2021)
Matthias Scheffler (resigned 26 November 2021)

Structure, governance and management

The organisation is governed by its Memorandum and Articles of Association dated 29 November 2007 and is a registered company limited by guarantee.

Psi-k is a Europe-based, worldwide network of researchers working on the advancement of first-principles computational materials science. Its mission is to develop fundamental theory, algorithms, and computer codes in order to understand, predict, and design materials properties and functions. Theoretical condensed matter physics, quantum chemistry, thermodynamics, and statistical mechanics form its scientific core. Applications encompass inorganic, organic and bio-materials, and cover a whole range of diverse scientific, engineering, and industrial endeavours. Key activities of Psi-k are the organisation of conferences, workshops, tutorials and training schools as well as the dissemination of scientific thinking in society.

Psi-k has a minimum of three Trustees, but there is no maximum. On the date of this report there were ten Trustees.

Psi-k has a Chair, and a Scientific Advisory Committee (SAC) of 81 members, which is headed by the Chair of Psi-k. In addition all Trustees are also SAC members.

The Board of Trustees meets on average five to six times a year, normally with a combination of face-to-face meetings and teleconference meetings. In 2021 there were six meetings, all by teleconference: on 4 February, 22 April, 24 June, 16 September, 21 October and 26 November (following the Annual Meeting of the SAC). Minutes of meetings are recorded, circulated, and kept for internal use. The Board of Trustees uses these meetings to discuss matters including but not limited to: future strategy, funding and finances, events such as workshops, conferences and summer schools, and relationships with external organisations such as CECAM.

PSI-K
(A COMPANY LIMITED BY GUARANTEE)
TRUSTEES' REPORT (CONTINUED)(INCLUDING DIRECTORS' REPORT)
FOR THE YEAR ENDED 31 DECEMBER 2021

The day to day running of Psi-k is delegated to the Chair, Peter Haynes, supported by the Operations Manager and Secretary, Damian Jones.

The SAC meets once a year, normally in November, together with the leaders of the 16 Working Group (<https://psi-k.net/groups/>). It is chaired by the Chair of Psi-k and its role is to make recommendations to the Board, particularly regarding plans for all activities for the following year (in this case, from Apr 2022 to March 2023). In 2021 the Annual Meeting was held online on 26 November.

For the second time in 2021, the Annual Meeting of the SAC was preceded by an open community meeting that was held online and advertised via the Psi-k mailing list.

All Trustees gave their time freely and no Trustee remuneration was paid in the year: expenses paid to Trustees amounted to €nil. Trustees are required to disclose all relevant interests and register them with the Chair.

Trustees are required to declare any conflicts of interest at each meeting and these are recorded in the minutes. If a vote of the Trustees is required on a matter, a Trustee who has declared a conflict of interest on that matter may not cast a vote.

Trustee training and induction process

The Trustees are chosen among members of the Scientific Advisory Council, that have thus been exposed to Psi-k activities and functioning for years. Each new Trustee discussed its role and responsibilities with the Chair.

Trustees are required to declare any conflicts of interest at each meeting and these are recorded in the minutes.

If a vote of the Trustees is required on a matter, a Trustee who has declared a conflict of interest on that matter may not cast a vote.

Reserves policy

It is the policy of the charity to maintain sufficient free reserves to fund their annual grants programme and cover the annual expenses. The trusts consider that the most appropriate level of free reserves in the long term is €200,000. Free reserves at 31 December 2021 are €338,955 (2020: €185,557).

Risk management

The Trustees have considered the major risks to which the charity is exposed and have reviewed those risks and established systems and procedures to manage those risks.

A significant risk for the Psi-k Charity is reduced financial funding. Since 2016, Psi-k has been sustained entirely by donations. In 2021 the Trustees agreed that our annual expenditure on community activities is determined by our income from the previous year, and adopted a target for reserves of €200,000. The Trustees have carefully considered the financial risks associated with the quinquennial Conference and consider them to be acceptable in view of the community benefit arising from a large, in-person conference, particularly for early career researchers and PhD students.

Objectives and activities

Europe has become the leading research area in the world for the application of first-principles computational modelling to materials science and Psi-k aims to maintain and enhance this status.

"Psi-k research" covers structures, properties and processes in all types of materials at the atomic level and in nanometre-scale structures, studied by ab initio quantum-mechanical computer simulation. A series of working groups represent the views of the community and organise activities to deliver the Psi-k mission:

PSI-K
(A COMPANY LIMITED BY GUARANTEE)
TRUSTEES' REPORT (CONTINUED)(INCLUDING DIRECTORS' REPORT)
FOR THE YEAR ENDED 31 DECEMBER 2021

Theme A: Physical Formalisms	
WG A1	Density and density-matrix functional theories
WG A2	Perturbative many-body methods
WG A3	Non-perturbative many-body methods
WG A4	Open and non-equilibrium systems
WG A5	Quasi-particle interactions and spectroscopies
Theme B: Algorithms, Software and Data	
WG B1	Reduced-scaling methods
WG B2	Statistics and configuration sampling
WG B3	Bridging length- and time-scales
WG B4	Software engineering
WG B5	High-throughput screening and data analytics
Theme C: Applications to Real Materials and Materials Design	
WG C1	Structural materials
WG C2	Functional materials and devices
WG C3	Magnetism and spintronics
WG C4	Surfaces and interfaces
WG C5	Nanoscale structures (2D, 1D, 0D) and related phenomena
WG C6	Molecules, macromolecules and biomolecules

Psi-k will promote and coordinate collaboration within the European research community by, among others, the following measures:

- supporting workshops and small conferences on specific topics of active research;
- supporting summer schools, tutorial courses and other training activities for young and new researchers in the field;
- organising a large "Psi-k conference" (such as those previously held in 1996, 2000, 2005, 2010 and 2015) every five years, although the next one has been postponed to August 2022 at EPFL in Switzerland;
- disseminating information about research progress, job opportunities, relevant workshops, conferences and other events, and funding opportunities via the Psi-k website providing a portal and a newsletter available freely to anyone in the world by electronic means.

The activities are open to all researchers in the field. Psi-k acts as a vehicle to engaging with the wider scientific community, with industry, European policy makers and trans-European computer centres. It will seek to maintain cooperation with organisations such as the Centre Européen de Calcul Atomique et Moléculaire (CECAM), the European molecular simulation community and its networks and Psi-k's counterpart research communities on other continents.

Aims and objectives for 2021

The main activities planned during 2021 comprised the scientific programme of workshops, conferences, tutorials and summer schools on the electronic structure of complex processes in materials, i.e. the topic of the Psi-k Charity, together with the Psi-k/CECAM Research Conference postponed from 2020. The pandemic caused some disruption to the 2021 programme: of just over 30 events, about half were delivered fully online, three in hybrid mode and seven fully in person. Only three events were postponed to 2022 and a further three cancelled. The Volker Heine Young Investigator Award was also held online in 2021.

PSI-K
(A COMPANY LIMITED BY GUARANTEE)
TRUSTEES' REPORT (CONTINUED)(INCLUDING DIRECTORS' REPORT)
FOR THE YEAR ENDED 31 DECEMBER 2021

Grant making policy

The Psi-k Charity does not make grants to other research bodies.

The Psi-k Charity applies its funding to the organization of workshops, summer schools, hands-on courses and the Psi-k Conference. The Theoretical and Computational Physics Group at STFC Daresbury Laboratory publishes the Psi-k Newsletter and provides administrative support.

The achievements of every workshop to which Psi-k contributes are monitored in the form of a report which is published on the Psi-k website (<http://psi-k.net/>).

Key performance indicators

In 2021 the Psi-k Charity organised 25 workshops, conferences and training activities (2020: nine). This is less than a normal year but a very significant increase from the number delivered in 2020.

Financial review 2021 and plan for 2022

Total donations receivable in 2021 have increased from the previous year to €207,621 (2020: €159,476). Member donations receivable were up slightly from the previous year, being €123,600 (2020: €122,000).

The expenses in the 2021 budget included €87,342 for workshops (2020: €148,500), €15,000 for the Psi-k/CECAM Conference (2020: €15,000) and €Nil (2020: €100,000) for the quinquennial Psi-k Conference, leading to total expenses of about €102,342 (2020: €263,500). However, due to a number of events moving online last year, the actual expenses for the year were €54,223 (2020: €60,310).

At the year end the net assets comprise debtors of € 35,825 (2020: €32,407) and bank balances €471,443 (2020: €351,875) less grant commitment creditors & accruals of €168,313 (2020: €198,725).

Plan for 2022: The Trustees are actively seeking new contributors with an aim of increasing annual members donations to around €150,000. The amount of €102,745 will be spent for workshops in 2022. Any deficit will be covered by the reserves.

During the year 2021 the Trustees were satisfied that, as far as circumstances permitted, the Charity continued to benefit the public through its activities targeted to achieve its charitable objectives.

Public Benefit

The Trustees confirm that they have referred to the guidance contained in the Charity Commission's general guidance on public benefit when reviewing the Trust's aims and objectives and in planning future activities and setting the grant making policy for the year.

PSI-K
(A COMPANY LIMITED BY GUARANTEE)
TRUSTEES' REPORT (CONTINUED)(INCLUDING DIRECTORS' REPORT)
FOR THE YEAR ENDED 31 DECEMBER 2021

Trustees' responsibilities

The Trustees (who are also Directors of Psi-k for the purposes of company law) are responsible for preparing the Trustees' Annual Report and the financial statements in accordance with applicable law and United Kingdom Accounting Standards (United Kingdom Generally Accepted Accounting Practice).

Company Law requires the Trustees to prepare financial statements for each financial year which give a true and fair view of the state of affairs of the charitable company and of the incoming resources and applications of resources, including the income and expenditure, of the charitable company for that year. In preparing those financial statements, the Trustees are required to:

- provide statements on the going concern basis unless it is inappropriate to presume that the charitable company will continue in business;
- select suitable accounting policies and apply them consistently;
- observe the methods and principles in the Charitable SORP;
- make judgements and estimates that are reasonable and prudent;
- state whether applicable accounting standards have been followed, subject to any material departures disclosed and explained in the financial statements.

The Trustees are responsible for keeping proper accounting records that disclose with reasonable accuracy at any time the financial position of the charitable company and enable them to ensure that the financial statements comply with the Companies Act 2006. They are also responsible for safeguarding the assets of the charitable company and hence for taking reasonable steps for the prevention of fraud and other irregularities.

This report has been prepared in accordance with the Statement of Recommended Practice: Accounting and Reporting by Charities (issued in March 2005) and in accordance with the special provisions applicable to small companies.

The trustees' report was approved by the Board of Trustees.



.....
Peter Haynes (Chair Person)

Trustee
Dated: 01/11/22

PSI-K
(A COMPANY LIMITED BY GUARANTEE)
INDEPENDENT EXAMINER'S REPORT
TO THE TRUSTEES OF PSI-K

I report to the trustees on my examination of the financial statements of the charity for the year ended 31 December 2021, which are set out on pages 1 to 17.

Respective responsibilities of trustees and examiner

As the trustees of the company (and also its directors for the purposes of company law) you are responsible for the preparation of the accounts in accordance with the requirements of the Companies Act 2006 ('the 2006 Act').

Having satisfied myself that the accounts of the company are not required to be audited under Part 16 of the 2006 Act and are eligible for independent examination I report in respect of my examination of your charity's accounts as carried out under section 145 of the Charities Act 2011 ('the 2011 Act'). In carrying out my examination I have followed the Directions given by the Charity Commission under section 145 (5)(b) of the 2011 Act.

An independent examination does not involve gathering all the evidence that would be required in an audit and consequently does not cover all the matters that an auditor considers in giving their opinion on the accounts. The planning and conduct of an audit goes beyond the limited assurance that an independent examination can provide. Consequently, I express no opinion as to whether the accounts present a 'true and fair view' and my report is limited to those specific matters set out in the independent examiner's statement.

Basis of independent examiner's report

I have completed my examination. I confirm that no material matters have come to my attention in connection with the examination giving me reasonable cause to believe that in any material respect:

1. accounting records were not kept in respect of the company as required by section 386 of the 2006 Act; or
2. the accounts do not accord with those records; or
3. the accounts do not comply with the accounting requirements of section 396 of the 2006 Act other than any requirement that the accounts give a 'true and fair view' which is not a matter considered as part of an independent examination; or
4. the accounts have not been prepared in accordance with the methods and principles of the Statement of Recommended Practice: Accounting and Reporting by Charities applicable to charities preparing their accounts in accordance with the Financial Reporting Standard applicable in the UK and Ireland (FRS 102).

I have no concerns and have come across no other matters in connection with the examination to which attention should be drawn in this report in order to enable a proper understanding of the accounts to be reached.

John Guest

Name: John Guest

Name of applicable listed body: The Institute of Chartered Accountants in England and Wales

Relevant professional qualification or membership of professional body: Chartered Accountant

ON BEHALF OF RSM UK TAX AND ACCOUNTING LIMITED

Chartered Accountants
5th Floor
One City Place
Queens Road
Chester
CH1 3BQ

Dated: 02/11/22

PSI-K
(A COMPANY LIMITED BY GUARANTEE)
STATEMENT OF FINANCIAL ACTIVITIES
INCLUDING INCOME AND EXPENDITURE ACCOUNT
FOR THE YEAR ENDED 31 DECEMBER 2021

	Notes	2021 €	2020 €
<u>Income from:</u>			
Donations and legacies	3	37,364	37,364
Charitable activities	4	170,257	122,112
Total income		207,621	159,476
<u>Expenditure on:</u>			
<u>Charitable activities</u>			
Grant Funding of Activities	5	54,223	60,310
Total charitable expenditure		54,223	60,310
Net income and net movement in funds for the year		153,398	99,166
Total funds brought forward		185,557	86,391
Total funds carried forward	13	338,955	185,557

The statement of financial activities includes all gains and losses recognised in the year.

All income and expenditure derive from continuing activities and are attributed to unrestricted funds.

The statement of financial activities also complies with the requirements for an income and expenditure account under the Companies Act 2006.

PSI-K
(A COMPANY LIMITED BY GUARANTEE)
BALANCE SHEET
AS AT 31 DECEMBER 2021

	Notes	2021 €	€	2020 €	€
Current assets					
Debtors	10	35,825		32,407	
Cash at bank and in hand		471,443		351,875	
		<u>507,268</u>		<u>384,282</u>	
Creditors: amounts falling due within one year	11	(168,313)		(198,725)	
Net current assets			338,955		185,557
Income funds					
Restricted funds			-		-
Unrestricted funds	13		338,955		185,557
			<u>338,955</u>		<u>185,557</u>

The company is entitled to the exemption from the audit requirement contained in section 477 of the Companies Act 2006, for the year ended 31 December 2021.

No member of the company has deposited a notice, pursuant to section 476, requiring an audit of these financial statements.

The directors acknowledge their responsibilities for:

- ensuring that the company keeps accounting records which comply with Section 396 of the Companies Act 2006; and
- preparing financial statements which give a true and fair view of the state of affairs of the company as at the end of each financial year and of its profit or loss for each financial year in accordance with the requirements of Section 396 and which otherwise comply with the requirements of the Companies Act 2006 relating to financial statements, so far as applicable to the company.

These financial statements have been prepared in accordance with the provisions applicable to companies subject to the small companies' regime and in accordance with Charities SORP (FRS102).

The notes on pages 9 to 17 form part of these accounts.

The financial statements were approved by the Trustees and authorised for issue on 01/11/22 and were signed on their behalf by:



Peter Haynes (Chair Person)
Trustee

PSI-K
(A COMPANY LIMITED BY GUARANTEE)
NOTES TO THE FINANCIAL STATEMENTS
FOR THE YEAR ENDED 31 DECEMBER 2021

1 Accounting policies

Charity information

PSI-K is a private company limited by guarantee incorporated in England and Wales. The registered office is Stfc Scitech Daresbury, Daresbury, Warrington, WA4 4AD.

Accounting convention

The financial statements have been prepared in accordance with Accounting and Reporting by Charities: Statement of Recommended Practice applicable to charities preparing their accounts in accordance with the Financial Reporting Standard applicable in the UK and Republic of Ireland (FRS102) (Issued October 2019)- (Charities SORP (FRS102)), the Financial Reporting Standard applicable to the UK and Republic of Ireland (FRS102) and the Companies Act 2006.

The financial statements are prepared in Euro and amounts in these financial statements are rounded to the nearest Euro.

PSI-K meets the definition of a public benefit entity under FRS 102. Assets and liabilities are initially recognised at historical cost or transaction value unless otherwise stated in the relevant accounting policy notes. The Charity has taken advantage of the provision in the SORP for the Charities applying FRS 102 Update Bulletin 1 not to prepare a Statement of Cash Flows.

Going concern

The trustees forecast that the charity will continue to be able to pay its liabilities as they fall due for a period of at least 12 months following the date of approving the financial statements. The forecasts take into account transactions that are anticipated to take place in the foreseeable future and indicate that no additional financial resources will be required should the actual performance differ from forecast. On this basis the trustees have concluded that adopting the going concern basis of accounting in preparing the annual financial statements is appropriate.

Charitable funds

Unrestricted funds are available for use at the discretion of the Trustees in furtherance of the general objectives of the Charity.

Restricted funds are to be used for specified purposes as laid down by the donor. Expenditure which meets these criteria is identified to the fund, together with a fair allocation of management and support costs.

Incoming resources

Incoming resources represents donations from research bodies in Europe to support the company's activities, less amounts carried forward to future periods as deferred income; and donated services, which are included based on the hours worked and the appropriate hourly rate. Income is recognised when the entity has entitlement to the funds, it is probable that the income will be received and the amount can be measured reliably.

Donated services

Donated services are included within incoming resources with an equivalent amount shown within resources expended, where the benefit to the charity is reasonably quantifiable, measurable and material. The value placed on these resources is the estimated value to the charity of the service received.

Deferred income

Donations received in advance of the period that they relate to, or which are provided specifically for future periods, are carried forward as deferred income. These amounts relate to contributions from research bodies received in advance.

PSI-K
(A COMPANY LIMITED BY GUARANTEE)
NOTES TO THE FINANCIAL STATEMENTS (CONTINUED)
FOR THE YEAR ENDED 31 DECEMBER 2021

1 Accounting policies (Continued)

Resources expended

All expenditure is accounted for on an accruals basis, inclusive of any VAT which cannot be recovered.

Grants payable are payments made to third parties in the furtherance of the charitable objectives of the Charity. Grants are accounted for when either the recipient has a reasonable expectation that they will receive a grant and the trustees have agreed to pay the grant without condition, or the recipient has a reasonable expectation that they will receive a grant and any condition attaching to the grant is outside of the control of the Charity.

Provisions for grants are made when the intention to make a grant has been communicated to the recipient but there is uncertainty about either the timing of the grant or the amount of grant payable.

Governance costs are related to the governance of the charity, such as the costs of preparing the accounts and statutory compliance.

Irrecoverable VAT is charged as a cost against the activity for which the expenditure was incurred.

Financial instruments

The Charity has elected to apply the provisions of Section 11 'Basic Financial Instruments' and Section 12 'Other Financial Instruments Issues' of FRS 102, in full, to all of its financial instruments.

Financial assets and financial liabilities are recognised when the Charity becomes a party to the contractual provisions of the instrument, and are offset only when the Charity currently has a legally enforceable right to set off the recognised amounts and intends either to settle on a net basis, or to realise the asset and settle the liability simultaneously.

Basic financial assets

Trade and other debtors (including accrued income) which are receivable within one year and which do not constitute a financing transaction are initially measured at the transaction price and subsequently measured at amortised cost, being the transaction price less any amounts settled and any impairment losses.

Basic financial liabilities

Financial instruments are classified as liabilities according to the substance of the contractual arrangements entered into.

Trade and other creditors (including accruals) payable within one year that do not constitute a financing transaction are initially measured at the transaction price and subsequently measured at amortised cost, being the transaction price less any amounts settled.

Derecognition of financial liabilities

Financial liabilities are derecognised when the charity's contractual obligations expire or are discharged or cancelled.

Foreign exchange

The trustees consider that the functional currency of the charity is the Euro, as most transactions are denominated and are carried out in that currency.

Assets and liabilities denominated in other currencies are translated into Euros at the rate of exchange ruling at the balance sheet date. Transactions in other currencies are translated into Euros at the rate of exchange ruling at the date of the transaction. Exchange differences are taken into account in arriving at the net movement in funds in the Statement of Financial Activities.

At the balance sheet date the rate of exchange between Sterling and Euro was £1 equals €1.1893 (2020: €1.1166).

PSI-K
(A COMPANY LIMITED BY GUARANTEE)
NOTES TO THE FINANCIAL STATEMENTS (CONTINUED)
FOR THE YEAR ENDED 31 DECEMBER 2021

2 Critical accounting estimates and judgements

In the application of the charity's accounting policies, the trustees are required to make judgements, estimates and assumptions about the carrying amount of assets and liabilities that are not readily apparent from other sources. The estimates and associated assumptions are based on historical experience and other factors that are considered to be relevant. Actual results may differ from these estimates.

The estimates and underlying assumptions are reviewed on an on-going basis. Revisions to accounting estimates are recognised in the period in which the estimate is revised where the revision affects only that period, or in the period of the revision and future periods where the revision affects both current and future periods.

No critical accounting estimates and judgements have been made in preparing these financial statements

3 Donations and legacies

	2021	2020
	€	€
Donated services	37,364	37,364
	<u> </u>	<u> </u>

Donations received from research bodies attributable to overseas markets totals 97% (2020: 87%). All income received in 2021 (and 2020) was unrestricted

4 Charitable activities

	2021	2020
	€	€
Donations from research bodies	170,257	122,112
	<u> </u>	<u> </u>

All income received in 2021 (and 2020) was unrestricted

PSI-K
(A COMPANY LIMITED BY GUARANTEE)
NOTES TO THE FINANCIAL STATEMENTS (CONTINUED)
FOR THE YEAR ENDED 31 DECEMBER 2021

5 Charitable activities

	2021	2020
	€	€
Exchange (gains)/losses	(1,189)	705
Grant funding of activities (see note 9)	8,077	9,636
Prize giving awards	2,000	-
Share of support costs (see note 6)	38,223	41,735
Share of governance costs (see note 6)	7,112	8,234
	<u>54,223</u>	<u>60,310</u>

Total expenditure for the year was €54,223, all of which was unrestricted expenditure (2020: €60,310). The grant funding of activities totalling €8,077 (2020: €9,636) relates to payments made to institutions regarding scientific conferences.

6 Support costs

	Support costs	Governance costs	2021	2020
	€	€	€	€
Bank charges	621	-	621	441
Donated services	37,364	-	37,364	37,364
Other support costs	-	-	-	3,930
Tax charge	238	-	238	-
Accountancy	-	2,048	2,048	5,212
Independent examination	-	3,926	3,926	3,022
Corporate tax	-	1,138	1,138	-
	<u>38,223</u>	<u>7,112</u>	<u>45,335</u>	<u>49,969</u>

It is estimated that the charity benefited from approximately 636 (2020: 636) hours of donated time provided to assist with the running of the charity. This figure was made up of 477 (2020: 477) hours of donated time received as a contribution in kind from the CCP9 service level agreement, and 159 (2020: 159) hours from the Science and Technology Facilities Council.

7 Staff costs

There were no employees during the year.

No employees received employee benefits over €70,000.

The Trustees were not paid any remuneration and so there is no remuneration paid to key management personnel.

Expenses of €Nil (2020: €600) were reimbursed to a trustee during the year relating to travel costs. As at 31 December 2021 there is a balance owed of €Nil (2020: €Nil).

PSI-K
(A COMPANY LIMITED BY GUARANTEE)
NOTES TO THE FINANCIAL STATEMENTS (CONTINUED)
FOR THE YEAR ENDED 31 DECEMBER 2021

8 Taxation

PSI-K is a registered charity and is therefore exempt from tax on its charitable income.

9 Grants payable

	2021	2020
	€	€
Grants to institutions:		
Linköping University, Sweden	-	5,000
CECAM, Luasanne	4,000	3,900
Fritz-Haber-Institut, Berlin	-	16,800
East African Institute for Fundamental Research, RWANDA	-	5,750
EPFL, Switzerland	3,600	2,000
CEA, Bruyere-le-Chatel, France	-	6,500
Italian Institute of Technology, Italy	-	8,000
Technical University of Denmark	-	5,000
SISSA, Italy	-	5,000
University of Latvia, Latvia	-	10,500
ARAID Foundation, Spain	-	11,000
University of North Texas, USA	-	3,000
Materials Center Leoben, Austria	-	4,833
Addis Ababa University, Ethiopia	-	6,759
Various Online Events	-	27,700
Hermes summer school 2018	-	600
Aarhus Institute of Advanced Studies (AIAS), Aarhus University, Denmark	4,310	-
The Abdus Salam International Centre for Theoretical Physics, Trieste (IT)	10,000	-
Aachen, Germany	3,000	-
Guidel, France	4,500	-
ICTP Trieste (Italy)	5,000	-
Daresbury Laboratory, UK	4,860	-
Stockholm University, Stockholm, Sweden	9,000	-
Leuven, Belgium	12,000	-
Bordeaux, France	3,600	-
Erice (Italy)	4,000	-
University of Warwick, UK	3,600	-
Gran Sasso Science Institute, L'Aquila, Italy	8,400	-
Ekaterinburg, Russia	7,875	-
Benasque Center for Science (Benasque, Spain)	12,000	-
Castle Reinsburg near Günzburg/Germany	3,000	-
Total institutional grants	102,745	122,342

PSI-K
(A COMPANY LIMITED BY GUARANTEE)
NOTES TO THE FINANCIAL STATEMENTS (CONTINUED)
FOR THE YEAR ENDED 31 DECEMBER 2021

9 Grants payable (Continued)

Reconciliation of grants payable		
Grant commitments brought forward	177,516	304,546
Commitments made during the year	102,745	303,742
Grants reschedules from 2020	-	(182,000)
Hermes summer school 2018 late invoice	-	600
Physics by the lake additional 2018 grant	1,000	-
Grant commitments for the year	103,745	122,342
Prior year grants cancelled/ recovered/ refunded	(95,668)	(112,706)
Grants payable for the year	8,077	9,636
Grants paid in year	(48,359)	(151,866)
Grants to be refunded	12,800	15,200
Grants refunded in year	4,000	-
Grant commitments carried forward	154,034	177,516

10 Debtors

	2021	2020
	€	€
Amounts falling due within one year:		
Trade debtors	23,025	17,207
Other debtors	12,800	15,200
	35,825	32,407

11 Creditors: amounts falling due within one year

		2021	2020
	Notes	€	€
Grant commitments		154,034	177,516
Deferred income	12	7,000	6,000
Accruals		7,279	15,209
		168,313	198,725

PSI-K
(A COMPANY LIMITED BY GUARANTEE)
NOTES TO THE FINANCIAL STATEMENTS (CONTINUED)
FOR THE YEAR ENDED 31 DECEMBER 2021

12 Deferred income

	2021	2020
	€	€
Deferred income as at 1 January 2021	6,000	19,000
Received in year	7,000	6,000
Released in year	(6,000)	(19,000)
	<u>7,000</u>	<u>6,000</u>
Deferred income as at 31 December 2021	<u>7,000</u>	<u>6,000</u>

Deferred income comprises contributions from research bodies received pre 31 December 2021 (and 2020) which have been invoiced in advance.

13 Statement of funds

The movements on the funds of the charity were as follows:

	Balance at 1 January	Movement in funds		Balance at 31
	2021	Incoming	Resources	December 2021
	€	resources	expended	€
General fund	185,557	207,621	(54,223)	338,955
	<u>185,557</u>	<u>207,621</u>	<u>(54,223)</u>	<u>338,955</u>

The movement on the funds of the charity in 2020 were as follows:

	Balance at 1 January	Movement in funds		Balance at 31
	2020	Incoming	Resources	December 2020
	€	resources	expended	€
General fund	86,391	159,476	(60,310)	185,557
	<u>86,391</u>	<u>159,476</u>	<u>(60,310)</u>	<u>185,557</u>

All funds for the year ended 31 December 2021 and year ended 31 December 2020 relate to unrestricted reserves.

PSI-K
(A COMPANY LIMITED BY GUARANTEE)
NOTES TO THE FINANCIAL STATEMENTS (CONTINUED)
FOR THE YEAR ENDED 31 DECEMBER 2021

14 Analysis of net assets between funds

Total 2021
€

Fund balances at 31 December 2021 are represented by:

Current assets	507,268
Creditors: Amounts falling due within one year	(168,313)
	338,955

Total 2020
€

Fund balances at 31 December 2020 are represented by:

Current assets	384,282
Creditors: Amounts falling due within one year	(198,725)
	185,557

15 Guarantee Company and Liability of Members

Psi-k is a company limited by guarantee and therefore does not have any share capital. The liability of members is limited. In the event of the charity being wound up during a member's period of membership or within one year after ceasing to be a member, an amount not exceeding the sum of £1 may be required from that member towards the payment of the debts and liabilities of the company incurred before membership ceased and the costs of winding up.

At 31 December 2021, the company had 10 (2020: 13) members.

16 Related party transactions

There were no disclosable related party transactions during the current year.

PSI-K

England & Wales - Charity number 1126308

Accounts

Company registration number 06440198

PSI-K
(A company limited by guarantee)

REPORT AND UNAUDITED FINANCIAL STATEMENTS

YEAR ENDED 31 DECEMBER 2020

PSI-K
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YEAR ENDED 31 DECEMBER 2020

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**PSI-K
LEGAL AND ADMINISTRATIVE INFORMATION
YEAR ENDED 31 DECEMBER 2020**

Psi-k is a company limited by guarantee and a registered charity governed by its Memorandum and Articles of Association dated 29 November 2007.

Company registration number: 06440198

Charity registration number: 1126308

DIRECTORS AND TRUSTEES

The directors of the company are its Trustees for the purpose of Charity Law and throughout this report are collectively referred to as the Trustees. The Trustees who served during the period and to the date of this report are set on page 4.

SECRETARY

Mrs. T A A Kelly

REGISTERED AND PRINCIPAL OFFICE

Daresbury Laboratory
Daresbury Science and Innovation Campus
Daresbury
Warrington
Cheshire
WA4 4AD

ACCOUNTANTS

RSM UK Tax and Accounting Limited
Chartered Accountants
One City Place
Queens Road
Chester
CH1 3BQ

BANKERS

HSBC Bank Plc
11 Stamford New Road
Altrincham
Cheshire
WA14 1BW

**PSI-K
REPORT OF THE CHAIRMAN
YEAR ENDED 31 DECEMBER 2020**

2020 was a challenging year for Psi-k, but one that also demonstrated the underlying strength of the community and the potential for adversity to provide opportunities for innovation. Originally the major quinquennial Psi-k Conference had been planned to take place in Lausanne in September 2020 but this has now had to be postponed until August 2022. In view of the Conference, a reduced programme of 21 workshops, conferences, tutorials and summer schools was planned. Three of these were held in person during the first two months of the year, but of the remainder only one was cancelled and 14 were postponed to 2021. However six activities went ahead in an online format and the feedback received from these was very positive, noting in particular that it is easier for researchers where funding is in short supply to participate.

Three Psi-k highlights were published in March, September and October, which can be found at <https://psi-k.net/highlights/>, together with all those published from 1994 onwards. We are always keen and happy to showcase work that combines breadth and depth and is relevant to the Psi-k community; any suggested contributions can be discussed with leon.petit@stfc.ac.uk. We have maintained our informal agreement with npj Computational Materials that provides an opportunity for the publication of approved Psi-k highlights with a waiver of the article processing charge to ensure it is fully open access and consistent with funding body requirements. In addition we have begun discussions with IOP Electronic Structure about providing additional opportunities.

All these activities are supported by the generous donations of groups worldwide – 38 groups or institutions from 14 countries have contributed to the charity. Anyone (individuals, groups, organisations, companies) that would like to contribute can contact p.haynes@imperial.ac.uk and PSIK_ADMIN@stfc.ac.uk.

The Working Groups were reorganised in 2017 and remain instrumental in coordinating the scientific programme. The 16 Working Groups are organised by three main themes, each overseen by a Trustee:

- A. Physical formalisms – Silke Biermann (École Polytechnique, Paris)
- B. Algorithms, software and data – Arash Mostofi (Imperial College London)
- C. Applications to real materials and materials design – Igor Abrikosov (Linköpings Universitet)

Further information about the Working Groups can be found at <https://psi-k.net/groups/>.

In 2020 the two-step submission process for workshop proposals continued, whereby a first deadline at the end of July is used for pre-proposals, which are light-touch submissions to be evaluated by the Working Groups and Trustees in order to coordinate and streamline all activities. Pre-proposals are either encouraged to submit a full proposal by the end of October, rejected right away, or advised to merge with other efforts on similar themes to avoid duplication. The CECAM Psi-k Research Conference has a separate application track, and any proposals not selected but deemed of sufficient quality can directly apply as a full proposal.

The Board of Trustees met six times in 2020, all by teleconference: on 21 January, 17 March, 22 May, 25 September, 21 October and 27 November. Minutes of meetings are recorded, circulated, and kept for internal use. The Trustees (<https://psi-k.net/admin/>), Working Group leaders (<https://psi-k.net/groups/>) and 25 members of the Scientific Advisory Committee (<https://psi-k.net/scientific-advisory-committee/>) attended the Annual Meeting on 27 November, where all activities are finalised for the following year (in this case, from April 2021 to March 2022). For the first time, an online community meeting was held before the Annual Meeting and advertised to the whole Psi-k mailing list. The Chair, Nicola Marzari, gave a presentation explaining how to get involved with Psi-k, and this was followed by a lively discussion.

PSI-K
REPORT OF THE CHAIRMAN (Continued)
YEAR ENDED 31 DECEMBER 2020

The generous contribution of time from all the groups above is essential to the wellbeing of the Charity, but particular thanks must go to Damian Jones (STFC Daresbury Laboratory, UK) for coordinating all the administration; to Peter Dederichs (Research Centre Jülich, Germany) our former Chair, who stepped down as a Trustee and Honorary Treasurer at the Annual Meeting after many years; and to Nicola Marzari, who stepped down as Chair after three years at the end of 2020. We are delighted that Peter and Nicola will continue their involvement in Psi-k: Peter as a member of the Scientific Advisory Committee and Nicola as a Trustee.

Peter Haynes - Psi-K Chair

P.D. Haynes

Date: 29 September 2021

**PSI-K
REPORT OF THE TRUSTEES
YEAR ENDED 31 DECEMBER 2020**

The Trustees present their annual report and unaudited financial Statements for the year ended 31 December 2020.

Trustees

The Trustees who served during the period and to the date of this report were:

Igor Abrikosov

Silke Biermann

Stefan Blügel

Peter Dederichs (Resigned 27 November 2020)

Claudia Draxl

Peter Haynes (Chair) (Appointed as chair on 1 January 2021)

Nicola Marzari (Resigned from the chair position on 31 December 2020)

Elisa Molinari

Arash Mostofi

Risto Nieminen

Mike Payne

Lucia Reining

Angel Rubio

Matthias Scheffler

Structure, governance and management

The organisation is governed by its Memorandum and Articles of Association and is a registered company limited by guarantee.

Psi-k is a Europe-based, worldwide network of researchers working on the advancement of first-principles computational materials science. Its mission is to develop fundamental theory, algorithms, and computer codes in order to understand, predict, and design materials properties and functions. Theoretical condensed matter physics, quantum chemistry, thermodynamics, and statistical mechanics form its scientific core. Applications encompass inorganic, organic and bio-materials, and cover a whole range of diverse scientific, engineering, and industrial endeavours. Key activities of Psi-k are the organisation of conferences, workshops, tutorials and training schools as well as the dissemination of scientific thinking in society.

Psi-k has a minimum of three Trustees, but there is no maximum. On the date of this report there were 13 Trustees.

Psi-k has a Chair, and a Scientific Advisory Committee (SAC) of 82 members, which is headed by the Chair of Psi-k. In addition all Trustees are also SAC members.

The Board of Trustees meets on average five to six times a year, normally with a combination of face-to-face meetings and teleconference meetings. In 2020 there were six meetings, all by teleconference: on 21 January, 17 March, 22 May, 25 September, 21 October and 27 November (following the Annual Meeting of the SAC). Minutes of meetings are recorded, circulated, and kept for internal use. The Board of Trustees uses these meetings to discuss matters including but not limited to: future strategy, funding and finances, events such as workshops, conferences and summer schools, and relationships with external organisations such as CECAM.

The day to day running of Psi-k is delegated to the Chair Nicola Marzari, who resigned with effect from 31 December but remains a Trustee. The Chair from 2021 is Peter Haynes.

The SAC meets once a year, normally in November, together with the leaders of the 16 Working Group (<https://psi-k.net/groups/>). It is chaired by the Chair of Psi-k and its role is to make recommendations to the Board, particularly regarding plans for all activities for the following year (in this case, from Apr 2021 to March 2022). In 2020 the Annual Meeting was held online on 27 November.

For the first time in 2020, the Annual Meeting of the SAC was preceded by an open community meeting that was held online and advertised via the Psi-k mailing list.

All Trustees gave their time freely and no Trustee remuneration was paid in the year: expenses paid to Trustees amounted to €600. Trustees are required to disclose all relevant interests and register them with the Chair.

These unaudited financial statements have been subjected to independent examination. See report on page 8.

**PSI-K
REPORT OF THE TRUSTEES
YEAR ENDED 31 DECEMBER 2020**

Trustees are required to declare any conflicts of interest at each meeting and these are recorded in the minutes. If a vote of the Trustees is required on a matter, a Trustee who has declared a conflict of interest on that matter may not cast a vote.

Trustee training and induction process

The Trustees are chosen among members of the Scientific Advisory Council, that have thus been exposed to Psi-k activities and functioning for years. Each new Trustee discussed its role and responsibilities with the Chair.

Trustees are required to declare any conflicts of interest at each meeting and these are recorded in the minutes. If a vote of the Trustees is required on a matter, a Trustee who has declared a conflict of interest on that matter may not cast a vote.

Reserve's policy

It is the policy of the charity to maintain sufficient free reserves to fund their annual grants programme and cover the annual expenses. The trusts consider that the most appropriate level of free reserves in the long term is 200,000 Euros.

Risk management

The Trustees have considered the major risks to which the charity is exposed and have reviewed those risks and established systems and procedures to manage those risks.

The largest risk for the Psi-k Charity is reduced financial funding. Since 2016, Psi-k has been sustained entirely by donations. Our annual expenditure on community activities exceeds our annual income from donations by about 50,000 Euros per year, which means that we are drawing down on our reserves of 350,000 Euros. Unless we rebalance things within a three-to-five year timeframe, this is one of the main risks to maintaining our activities at the current level and also an obstacle to growth of activities.

Objectives and activities

Europe has become the leading research area in the world for the application of first-principles computational modelling to materials science and Psi-k aims to maintain and enhance this status.

“Psi-k research” covers structures, properties and processes in all types of materials at the atomic level and in nanometre-scale structures, studied by ab initio quantum-mechanical computer simulation. A series of working groups represent the views of the community and organise activities to deliver the Psi-k mission:

Theme A: Physical Formalisms	
WG A1	Density and density-matrix functional theories
WG A2	Perturbative many-body methods
WG A3	Non-perturbative many-body methods
WG A4	Open and non-equilibrium systems
WG A5	Quasi-particle interactions and spectroscopies
Theme B: Algorithms, Software and Data	
WG B1	Reduced-scaling methods
WG B2	Statistics and configuration sampling
WG B3	Bridging length- and time-scales
WG B4	Software engineering
WG B5	High-throughput screening and data analytics
Theme C: Applications to Real Materials and Materials Design	
WG C1	Structural materials
WG C2	Functional materials and devices
WG C3	Magnetism and spintronics
WG C4	Surfaces and interfaces
WG C5	Nanoscale structures (2D, 1D, 0D) and related phenomena
WG C6	Molecules, macromolecules and biomolecules

These unaudited financial statements have been subjected to independent examination. See report on page 8.

**PSI-K
REPORT OF THE TRUSTEES
YEAR ENDED 31 DECEMBER 2020**

Psi-k will promote and coordinate collaboration within the European research community by, among others, the following measures:

- supporting workshops and small conferences on specific topics of active research;
- supporting summer schools, tutorial courses and other training activities for young and new researchers in the field;
- organising a large “Psi-k conference” (such as those previously held in 1996, 2000, 2005, 2010 and 2015) every five years, although the next one has been postponed to August 2022 at EPFL in Switzerland;
- disseminating information about research progress, job opportunities, relevant workshops, conferences and other events, and funding opportunities via the Psi-k website providing a portal and a newsletter available freely to anyone in the world by electronic means.

The activities are open to all researchers in the field. Psi-k acts as a vehicle to engaging with the wider scientific community, with industry, European policy makers and trans-European computer centres. It will seek to maintain cooperation with organisations such as the Centre Européen de Calcul Atomique et Moléculaire (CECAM), the European molecular simulation community and its networks and Psi-k’s counterpart research communities on other continents.

Aims and objectives for 2020

The main activities planned during 2020 comprised the scientific programme of workshops, conferences, tutorials and summer schools on the electronic structure of complex processes in materials, i.e. the topic of the Psi-k Charity, together with the Psi-k 2020 general conference. The pandemic caused severe disruption to the 2020 programme: three workshops were held in person as planned during the first two months of the year, but of 21 other activities scheduled for the year, only one was cancelled, with six delivered online and 14 postponed to 2021. This does not include the 2020 Psi-k Conference that has been postponed to August 2022.

Grant making policy

The Psi-k Charity does not make grants to other research bodies.

The Psi-k Charity applies its funding to the organization of workshops, summer schools, hands-on courses and the Psi-k Conference. The Theoretical and Computational Physics Group at STFC Daresbury Laboratory publishes the Psi-k Newsletter and provides administrative support.

The achievements of every workshop to which Psi-k contributes are monitored in the form of a report which is published on the Psi-k website (<http://psi-k.net/>).

Key performance indicators

In 2020 the Psi-k Charity organised only nine workshops, conferences and training activities. This is less than a third of those organised in 2019, although there are normally fewer of these activities in the year of the Psi-k Conference. Fourteen of these activities have been postponed to 2021. The Psi-k Conference also meant that there was no “Psi-k Scientific Get-Together” at the annual DPG Conference either.

Financial review 2020 and plan for 2021

Member donations in 2020 have decreased from the previous year, with a total of 159,476 Euros received (2019: 186,145). The budgeted expenses in the 2020 included 148,500 Euros for workshops, 100,000 Euros for the quinquennial Psi-k Conference and 15,000 Euro for the Psi-k/CECAM Conference amounting to total budgeted expenses of 263,500 Euros. However, a large number of these events were either cancelled or postponed to 2021 due to the pandemic, and actual expenditure for 2020 was therefore reduced to 60,310 Euro (2019: 332,785 Euro), resulting in a surplus for the year of 99,166 Euro (2019: deficit of 146,640 Euro).

Plan for 2021: The Trustees are actively seeking new contributors and we have recently added a PayPal option via the Psi-k website to make donating easier. We hope to increase the annual donations to approximately 150,000 Euros. An amount of 102,342 Euros will be spent on workshops in 2021, and in addition 15,000 Euros will be spent on the CECAM/Psi-k Conference postponed from 2020, along with several other events postponed from 2020. This will give us total expected expenses for 2021 of approximately 200,000 Euros. Any deficit resulting from additional activities in 2021 will be covered by the charities cash reserves.

During the year 2020 the Trustees were satisfied that, as far as circumstances permitted, the Charity continued to benefit the public through its activities targeted to achieve its charitable objectives.

These unaudited financial statements have been subjected to independent examination. See report on page 8.

**PSI-K
REPORT OF THE TRUSTEES
YEAR ENDED 31 DECEMBER 2020**

Public Benefit

The Trustees confirm that they have referred to the guidance contained in the Charity Commission's general guidance on public benefit when reviewing the Trust's aims and objectives and in planning future activities and setting the grant making policy for the year.

Trustee's responsibilities

The Trustees (who are also Directors of Psi-k for the purposes of company law) are responsible for preparing the Trustees' Annual Report and the financial statements in accordance with applicable law and United Kingdom Accounting Standards (United Kingdom Generally Accepted Accounting Practice).

Company Law requires the Trustees to prepare financial statements for each financial year which give a true and fair view of the state of affairs of the charitable company and of the incoming resources and applications of resources, including the income and expenditure, of the charitable company for that year. In preparing those financial statements, the Trustees are required to:

- provide statements on the going concern basis unless it is inappropriate to presume that the charitable company will continue in business;
- select suitable accounting policies and apply them consistently;
- observe the methods and principles in the Charitable SORP;
- make judgements and estimates that are reasonable and prudent;
- state whether applicable accounting standards have been followed, subject to any material departures disclosed and explained in the financial statements.

The Trustees are responsible for keeping proper accounting records that disclose with reasonable accuracy at any time the financial position of the charitable company and enable them to ensure that the financial statements comply with the Companies Act 2006. They are also responsible for safeguarding the assets of the charitable company and hence for taking reasonable steps for the prevention of fraud and other irregularities.

This report has been prepared in accordance with the Statement of Recommended Practice: Accounting and Reporting by Charities (FRS 102) (Issued October 2019) - (Charities SORP (FRS 102) and in accordance with the special provisions applicable to small companies.

ON BEHALF OF THE BOARD

Peter Haynes

P.D. Haynes

Date: 29 September 2021

INDEPENDENT EXAMINER'S REPORT TO THE TRUSTEES OF PSI-K

I report to the trustees on my examination of the financial statements of PSI-K ("the company") for the year ended 31 December 2020, which are set out on pages 9 to 16.

Responsibilities and basis of report

As the trustees of the company (and also its directors for the purposes of company law) you are responsible for the preparation of the financial statements in accordance with the requirements of the Companies Act 2006 ('the 2006 Act').

Having satisfied myself that the financial statements of the company are not required to be audited under Part 16 of the 2006 Act and are eligible for independent examination I report in respect of my examination of your charity's financial statements as carried out under section 145 of the Charities Act 2011 ('the 2011 Act'). In carrying out my examination I have followed the Directions given by the Charity Commission under section 145 (5)(b) of the 2011 Act.

An independent examination does not involve gathering all the evidence that would be required in an audit and consequently does not cover all the matters that an auditor considers in giving their opinion on the financial statements. The planning and conduct of an audit goes beyond the limited assurance that an independent examination can provide. Consequently, I express no opinion as to whether the accounts present a 'true and fair view' and my report is limited to those specific matters set out in the independent examiner's statement.

Independent examiner's statement

I have completed my examination. I confirm that no material matters have come to my attention in connection with the examination giving me reasonable cause to believe that in any material respect:

1. accounting records were not kept in respect of the company as required by section 386 of the 2006 Act; or
2. the financial statements do not accord with those records; or
3. the financial statements do not comply with the accounting requirements of section 396 of the 2006 Act other than any requirement that the accounts give a 'true and fair view' which is not a matter considered as part of an independent examination; or
4. the financial statements have not been prepared in accordance with the methods and principles of the Statement of Recommended Practice: Accounting and Reporting by Charities applicable to charities preparing their accounts in accordance with the Financial Reporting Standard applicable in the UK and Ireland (FRS 102).

I have no concerns and have come across no other matters in connection with the examination to which attention should be drawn in this report in order to enable a proper understanding of the accounts to be reached.

RSM UK Tax and Accounting Limited

Name: **John Guest**

Name of applicable listed body: **The Institute of Chartered Accountants in England and Wales**

Relevant professional qualification or membership of professional body: **Chartered Accountant**

ON BEHALF OF RSM UK TAX AND ACCOUNTING LIMITED

Chartered Accountants

One City Place

Queens Road

Chester

CH1 3BQ

Date: 29 September 2021

PSI-K
STATEMENT OF FINANCIAL ACTIVITIES
INCLUDING INCOME AND EXPENDITURE ACCOUNT
YEAR ENDED 31 DECEMBER 2020

	Notes	Unrestricted Funds €	Restricted €	Total Funds 2020 €	Total Funds 2019 €
INCOME FROM:					
Donations					
- Donated services		37,364	-	37,364	37,364
Charitable activities					
- Donations from research bodies		122,112	-	122,112	148,781
TOTAL INCOME		<u>159,476</u>	<u>-</u>	<u>159,476</u>	<u>186,145</u>
EXPENDITURE ON:					
Charitable activities					
- Contributions to scientific conferences		59,605	-	59,605	333,814
- Exchange losses / (gains)		705	-	705	(1,029)
TOTAL EXPENDITURE	4	<u>60,310</u>	<u>-</u>	<u>60,310</u>	<u>332,785</u>
NET INCOME/(EXPENDITURE) AND NET MOVEMENT IN FUNDS FOR THE YEAR		<u>99,166</u>	<u>-</u>	<u>99,166</u>	<u>(146,640)</u>
RECONCILIATION OF FUNDS					
TOTAL FUNDS BROUGHT FORWARD		<u>86,391</u>	<u>-</u>	<u>86,391</u>	<u>233,031</u>
TOTAL FUNDS CARRIED FORWARD	12	<u><u>185,557</u></u>	<u><u>-</u></u>	<u><u>185,557</u></u>	<u><u>86,391</u></u>

The Statement of Financial Activities includes all gains and losses recognised in the year.

All income and expenditure derives from continuing activities.

**PSI-K
BALANCE SHEET
AS AT 31 DECEMBER 2020**

Company registration number 06440198

	Notes	2020 €	2019 €
CURRENT ASSETS			
Debtors	9	32,407	17,950
Cash at bank		351,875	398,961
		<u>384,282</u>	<u>416,911</u>
CREDITORS: Amounts falling due within one year			
	10	(198,725)	(330,520)
		<u></u>	<u></u>
TOTAL ASSETS LESS CURRENT LIABILITIES			
		<u>185,557</u>	<u>86,391</u>
FUNDS/			
Unrestricted	12	185,557	86,391
Restricted	12	-	-
		<u></u>	<u></u>
TOTAL CHARITY FUNDS			
	12	<u>185,557</u>	<u>86,391</u>

For the year ending 31 December 2020 the company was entitled to exemption from audit under Section 477 of the Companies Act 2006 relating to small companies.

The members have not required the company to obtain an audit of its financial statements for the year ended 31 December 2020 in accordance with Section 476 of the Companies Act 2006.

The directors acknowledge their responsibilities for:

- ensuring that the company keeps accounting records which comply with Section 396 of the Companies Act 2006; and
- preparing financial statements which give a true and fair view of the state of affairs of the company as at the end of each financial year and of its profit or loss for each financial year in accordance with the requirements of Section 396 and which otherwise comply with the requirements of the Companies Act 2006 relating to financial statements, so far as applicable to the company.

These financial statements are prepared in accordance with the provisions applicable to companies subject to the small companies regime and in accordance with Charities SORP (FRS102).

The notes on pages 11 to 16 form part of these accounts

The financial statements were approved by the Trustees and authorised for issue on 22 April 2021 and were signed on their behalf by:

P.D. Haynes
Peter Haynes

Trustee

These unaudited financial statements have been subjected to independent examination. See report on page 8.

PSI-K
NOTES TO THE FINANCIAL STATEMENTS
YEAR ENDED 31 DECEMBER 2020

1. ACCOUNTING POLICIES

a. Basis of preparation

The financial statements have been prepared in accordance with Accounting and Reporting by Charities: Statement of Recommended Practice applicable to charities preparing their accounts in accordance with the Financial Reporting Standard applicable in the UK and Republic of Ireland (FRS 102) (Issued October 2019) - (Charities SORP (FRS 102)), the Financial Reporting Standard applicable in the UK and Republic of Ireland (FRS 102) and the Companies Act 2006.

The financial statements are prepared in Euro and amounts in these financial statements are rounded to the nearest Euro.

PSI-K meets the definition of a public benefit entity under FRS 102. Assets and liabilities are initially recognised at historical cost or transaction value unless otherwise stated in the relevant accounting policy notes. The Charity has taken advantage of the provisions in the SORP for Charities applying FRS102 Update Bulletin 1 not to prepare a Statement of Cash Flows.

b. Preparation of the accounts on a going concern basis

The trustees forecast that the charity will continue to be able to pay its liabilities as they fall due for a period of at least 12 months following the date of approving the financial statements. The forecasts take into account transactions that are anticipated to take place in the foreseeable future and indicate that no additional financial resources will be required should the actual performance differ from forecast. On this basis the trustees have concluded that adopting the going concern basis of accounting in preparing the annual financial statements is appropriate.

c. Income recognition

Incoming resources represents donations from research bodies in Europe to support the company's activities, less amounts carried forward to future periods as deferred income; and donated services, which are included based on the hours worked and the appropriate hourly rate. Income is recognised when the entity has entitlement to the funds, it is probable that the income will be received and the amount can be measured reliably.

d. Donated services

Donated services are included within incoming resources with an equivalent amount shown within resources expended, where the benefit to the charity is reasonably quantifiable, measurable and material. The value placed on these resources is the estimated value to the charity of the service received.

e. Deferred income

Donations received in advance of the period that they relate to, or which are provided specifically for future periods, are carried forward as deferred income. These amounts relate to contributions from research bodies received in advance.

f. Expenditure recognition

All expenditure is accounted for on an accruals basis, inclusive of any VAT which cannot be recovered.

Grants payable are payments made to third parties in the furtherance of the charitable objectives of the Charity. Grants are accounted for when either the recipient has a reasonable expectation that they will receive a grant and the trustees have agreed to pay the grant without condition, or the recipient has a reasonable expectation that they will receive a grant and any condition attaching to the grant is outside of the control of the Charity.

Provisions for grants are made when the intention to make a grant has been communicated to the recipient but there is uncertainty about either the timing of the grant or the amount of grant payable.

Governance costs are related to the governance of the charity, such as the costs of preparing the accounts and statutory compliance.

Irrecoverable VAT is charged as a cost against the activity for which the expenditure was incurred.

PSI-K
NOTES TO THE FINANCIAL STATEMENTS
YEAR ENDED 31 DECEMBER 2020

1. ACCOUNTING POLICIES (Continued)

g. Funds

Restricted funds are to be used for specified purposes as laid down by the donor. Expenditure which meets these criteria is identified to the fund, together with a fair allocation of management and support costs.

Unrestricted funds are available for use at the discretion of the Trustees in furtherance of the general objectives of the Charity.

h. Foreign currencies

The trustees consider that the functional currency of the charity is the Euro, as most transactions are denominated and are carried out in that currency.

Assets and liabilities denominated in other currencies are translated into Euros at the rate of exchange ruling at the balance sheet date. Transactions in other currencies are translated into Euros at the rate of exchange ruling at the date of the transaction. Exchange differences are taken into account in arriving at the net movement in funds in the Statement of Financial Activities.

At the balance sheet date the rate of exchange between Sterling and Euro was £1 equals €1.1166 (2019: €1.1812).

i. Financial instruments

The Charity has elected to apply the provisions of Section 11 'Basic Financial Instruments' and Section 12 'Other Financial Instruments Issues' of FRS 102, in full, to all of its financial instruments.

Financial assets and financial liabilities are recognised when the Charity becomes a party to the contractual provisions of the instrument, and are offset only when the Charity currently has a legally enforceable right to set off the recognised amounts and intends either to settle on a net basis, or to realise the asset and settle the liability simultaneously.

j. Financial assets

Trade and other debtors (including accrued income) which are receivable within one year and which do not constitute a financing transaction are initially measured at the transaction price and subsequently measured at amortised cost, being the transaction price less any amounts settled and any impairment losses.

k. Financial liabilities

Financial instruments are classified as liabilities according to the substance of the contractual arrangements entered into.

Trade and other creditors (including accruals) payable within one year that do not constitute a financing transaction are initially measured at the transaction price and subsequently measured at amortised cost, being the transaction price less any amounts settled.

2. CRITICAL ACCOUNTING ESTIMATES AND JUDGMENT

In the application of the charity's accounting policies, the trustees are required to make judgements, estimates and assumptions about the carrying amount of assets and liabilities that are not readily apparent from other sources. The estimates and associated assumptions are based on historical experience and other factors that are considered to be relevant. Actual results may differ from these estimates.

The estimates and underlying assumptions are reviewed on an on-going basis. Revisions to accounting estimates are recognised in the period in which the estimate is revised where the revision affects only that period, or in the period of the revision and future periods where the revision affects both current and future periods.

No critical accounting estimates and judgements have been made in preparing these financial statements.

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NOTES TO THE FINANCIAL STATEMENTS
YEAR ENDED 31 DECEMBER 2020

3. INCOME

Donations received from research bodies attributable to overseas markets totals 87% (2019: 90%). All income received in 2020 was unrestricted.

4. TOTAL EXPENDITURE

	Grant Funding of Activities €	Support Costs €	Total 2020 €	Total 2019 €
Charitable Activities				
Contributions to scientific conferences (Note 8)	9,636	41,735	51,371	326,842
Exchange losses / (gains)	-	705	705	(1,029)
Governance Costs (Note 5)	-	8,234	8,234	6,972
	<u>9,636</u>	<u>50,674</u>	<u>60,310</u>	<u>332,785</u>

Total expenditure for the year was €60,310, all of which was unrestricted expenditure, (2019: €332,785).

The grant funding of activities totalling €9,636 (2019: €311,223) relates to payments made to institutions regarding scientific conferences.

	2020 €	2019 €
Support costs comprise:		
Bank charges	441	793
Donated services	37,364	37,364
Other support costs	3,930	36,199
	<u>41,735</u>	<u>74,365</u>

It is estimated that the charity benefited from approximately 636 (2019: 636) hours of donated time provided to assist with the running of the charity. This figure was made up of 477 (2019: 477) hours of donated time received as a contribution in kind from the CCP9 service level agreement, and 159 (2019: 159) hours from the Science and Technology Facilities Council.

5. GOVERNANCE COSTS

	Total 2020 €	Total 2019 €
Governance costs are made up of the following:		
Independent examiners fee	3,022	3,286
Accountancy	5,212	3,686
	<u>8,234</u>	<u>6,972</u>

6. STAFF COSTS

There were no employees in the year. No employees received employee benefits over €70,000.

The Trustees were not paid any remuneration and so there is no remuneration paid to key management personnel. Expenses of €600 were reimbursed to a trustee during the year relating to travel costs (2019: €337.50) at 31 December 2020 there is a balance owed of €nil (2019: €nil).

7. TAXATION

PSI-K is a registered charity and is therefore exempt from tax on its charitable income.

These unaudited financial statements have been subjected to independent examination. See report on page 8.

PSI-K
NOTES TO THE FINANCIAL STATEMENTS
YEAR ENDED 31 DECEMBER 2020

8. GRANTS MADE TO INSTITUTIONS	2020	2019
	€	€
Grants awarded in the year were all to institutions and comprised:		
University del Pais Vasco, Spain	-	4,000
Linköping University, Sweden	5,000	10,000
Ecole Polytechnique, France	-	3,000
CECAM, Lausanne	3,900	3,500
Fritz-Haber-Institut, Berlin	16,800	-
Kings College, London	-	3,500
Weizmann Institute of Science, Switzerland	-	5,000
East African Institute for Fundamental Research, RWANDA	5,750	-
EPFL, Switzerland	2,000	108,500
DTU Compute, Switzerland	-	6,000
CNR (Italian National Research Council), Rome	-	4,000
Aalto University, Finland	-	3,000
University of Bath, Italy	-	9,000
CEA, Bruyères-le-Châtel, France	6,500	-
Italian Institute of Technology, Italy	8,000	-
ICTP, Italy	-	16,500
Max Planck Institute for the Structure and Dynamics of Matter	-	11,000
Friedrich-Schiller-Universität Jena, Germany	-	-
Humboldt-Universität zu Berlin, Germany	-	16,000
Technical University of Denmark	5,000	10,000
SISSA, Italy	5,000	-
University of Latvia, Latvia	10,500	-
ARAID Foundation, Spain	11,000	-
Institute of Science, Switzerland	-	1,500
University of Bremen, Germany	-	5,500
University of Rome, Italy	-	11,500
London, UK	-	15,000
University of Cambridge, UK	-	5,000
University of North Texas, USA	3,000	-
Technical University Munich, Germany	-	4,500
Materials Centre Leoben, Austria	4,833	-
University of Montpellier, France	-	3,500
University of Oxford, UK	-	4,000
PSI-K Research conference	-	15,000
Addis Ababa University, Ethiopia	6,759	-
Various online events	27,700	-
Hermes summer school 2018	600	-
Total institutional grants	122,342	278,500
Reconciliation of grants payable		
Grant commitments brought forward	304,546	247,806
Commitments made during the year	303,742	278,500
Grants rescheduled from 2020	(182,000)	-
Hermes summer school 2018 late invoice	600	-
Grant commitments for the year	122,342	278,500
Grants cancelled or recovered	(112,706)	(26,014)
Grants payable for the year	9,636	252,486
Grants paid	(151,866)	(195,746)
Grants to be refunded	15,200	-
Grant commitments carried forward	177,516	304,546

These unaudited financial statements have been subjected to independent examination. See report on page 8.

PSI-K
NOTES TO THE FINANCIAL STATEMENTS
YEAR ENDED 31 DECEMBER 2020

9. DEBTORS	2020 €	2019 €
Trade debtors	17,207	17,950
Accrued income	-	-
Other debtors	15,200	
	<u>32,407</u>	<u>17,950</u>
10. CREDITORS: Amounts falling due within one year	2020 €	2019 €
Grant commitments	177,516	304,546
Accruals	15,209	6,974
Deferred income (note 11)	6,000	19,000
	<u>198,725</u>	<u>330,520</u>
11. DEFERRED INCOME	2020 €	
Deferred income as at 1 January 2020	19,000	
Received in year	6,000	
Released in year	(19,000)	
	<u>6,000</u>	
Deferred income as at 31 December 2020	<u>6,000</u>	

Deferred income comprises contributions from research bodies received pre 31 December 2020 which have been invoiced in advance.

12. STATEMENT OF FUNDS
The movements on the funds of the charity were as follows:

	Balance 01.01.20	Income	Expenditure	Transfer	Balance 31.12.30
	€	€	€	€	€
Restricted Funds					
Restricted funds	-	-	-	-	-
	<u>-</u>	<u>-</u>	<u>-</u>	<u>-</u>	<u>-</u>
Unrestricted Funds					
General Fund	86,391	159,476	(60,310)	-	185,557
	<u>86,391</u>	<u>159,476</u>	<u>(60,310)</u>	<u>-</u>	<u>185,557</u>
Total Funds	<u>86,391</u>	<u>159,476</u>	<u>(60,310)</u>	<u>-</u>	<u>185,557</u>

These unaudited financial statements have been subjected to independent examination. See report on page 8.

PSI-K
NOTES TO THE FINANCIAL STATEMENTS
YEAR ENDED 31 DECEMBER 2020

12. STATEMENT OF FUNDS (continued)

The movement on the funds of the charity in 2019 were as follows:

	Balance 01.01.19	Income	Expenditure	Transfer	Balance 31.12.19
	€	€	€	€	€
Restricted Funds					
Restricted funds	-	-	-	-	-
	<u>-</u>	<u>-</u>	<u>-</u>	<u>-</u>	<u>-</u>
	<u><u>-</u></u>	<u><u>-</u></u>	<u><u>-</u></u>	<u><u>-</u></u>	<u><u>-</u></u>
Unrestricted Funds					
General Fund	233,031	186,145	(332,785)	-	86,391
	<u>233,031</u>	<u>186,145</u>	<u>(332,785)</u>	<u>-</u>	<u>86,391</u>
	<u><u>233,031</u></u>	<u><u>186,145</u></u>	<u><u>(332,785)</u></u>	<u><u>-</u></u>	<u><u>86,391</u></u>
Total Funds	<u>233,031</u>	<u>186,145</u>	<u>(332,785)</u>	<u>-</u>	<u>86,391</u>
	<u><u>233,031</u></u>	<u><u>186,145</u></u>	<u><u>(332,785)</u></u>	<u><u>-</u></u>	<u><u>86,391</u></u>

13. ANALYSIS OF NET ASSETS BETWEEN FUNDS

	Unrestricted Funds €	Restricted Funds €	Total 2020 €
Fund balances at 31 December 2020 are represented by:			
Current assets	384,282	-	384,282
Creditors: Amounts falling due within one year	(198,725)	-	(198,725)
Total Net Assets	<u>185,557</u>	<u>-</u>	<u>185,557</u>
	<u><u>185,557</u></u>	<u><u>-</u></u>	<u><u>185,557</u></u>
	Unrestricted Funds €	Restricted Funds €	Total 2019 €
Fund balances at 31 December 2019 are represented by:			
Current assets	416,911	-	416,911
Creditors: Amounts falling due within one year	(330,520)	-	(330,520)
Total Net Assets	<u>86,391</u>	<u>-</u>	<u>86,391</u>
	<u><u>86,391</u></u>	<u><u>-</u></u>	<u><u>86,391</u></u>

14. GUARANTEE COMPANY AND LIABILITY OF MEMBERS

Psi-k is a company limited by guarantee and therefore does not have any share capital.

The liability of members is limited. In the event of the charity being wound up during a member's period of membership or within one year after ceasing to be a member, an amount not exceeding the sum of £1 may be required from that member towards the payment of the debts and liabilities of the company incurred before membership ceased and the costs of winding up.

At 31 December 2020, the company had 13 (2019: 14) members.

15. RELATED PARTY

There are deemed to be no related parties of the entity which require reporting during the year.

These unaudited financial statements have been subjected to independent examination. See report on page 8.