



Pre-proposals call for 2021-22 Psi-k activities

Psi-k is a 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. Key activities of Psi-k are the organization of conferences, workshops, tutorials and training schools as well as the dissemination of scientific thinking in society [Excerpt from the mission statement at <http://psi-k.net/>].

In normal years Psi-k typically funds schools (1-2 weeks), workshops (2-3 days), international conferences (2-5 days), and codes/methods tutorials (3 days-1 week), with a focus on electronic-structure methods, developments, and applications. Funding is of the order of 4,000/8,000/12,000 €, depending on size and duration (as a guideline, 30 €/expected participant/day); Psi-k funds around 25-35 activities for every call (see here <http://psi-k.net/workshops/> for the 2020-21 activities).

For this call, while we plan to support some of these more traditional activities, we also call for a renewed focus on, attention to and ingenious development of novel models in research sharing, dissemination, teaching, and discussion – the freedom of our Charity allows us to consider less conventional proposals with funding devoted to digital or remote approaches.

We have a two-step application process to simplify and streamline applications, elicit more original proposals, improve planning, and avoid duplication of efforts. The present call for pre-proposals is for events that will take place between 1 April 2021 and 31 March 2022.

Please note: for this year only events that take place in August and September 2021 will NOT be considered for funding to avoid a clash with the rescheduled Psi-k Conference that will take place in Lausanne, 23-27 August 2021.

Pre-proposals should be submitted online by **Friday 31 July 2020** (midnight UK time), describing the planned event (see below for a draft of the form). Psi-k Working Groups (<http://psi-k.net/groups>) and Trustees (<http://psi-k.net/admin/>) will either approve this pre-proposal for full submission, reject it, or suggest a merger between different activities – you are very welcome to contact the relevant Working Group leaders or members beforehand.

Feedback will be provided the week of **Monday 21 September 2020**. Pre-proposals that have been approved or mergers that have been successfully negotiated will then be invited to submit a full proposal by **Friday 30 October 2020**. These proposals will then be evaluated and approved - with full or partial funding - or declined at the meeting of the Trustees, Scientific Advisory Committee (<http://psi-k.net/scientific-advisory-committee/>) and Working Group leaders on **Friday 27 November 2020**.

The evaluation of the pre-proposals and full proposals will be based on

1. the scientific quality of the proposal,
2. its intellectual inclusiveness and diversity of representatives,
3. the scientific merit of the organizers, and
4. appropriateness of budget, while of course
5. responding to the Psi-k mission statement

NOTES

- *in case of events that can interest different Working Groups please name the primary Working Group and then any related groups*
- *if the event does not relate to any current Working Group, applicants should contact in advance Psi-k at PSIK_ADMIN@stfc.ac.uk.*

Personal Information

First Name:

Last Name:

Email Address:

Application Questions

Note: Questions marked with a * are mandatory.

*Event Title

*Event Kind

- School
- Workshop
- International Conference
- Code Tutorial
- Other

*Primary Contact Name

*Primary Contact Email

*Primary Contact Affiliation

*List the name, email and affiliation of all event co-organisers

*Location of Event

*Dates of Event

*Duration of Event (in days to the nearest half day)

*Expected Number of Participations

*Total Budget of Event (In EUROS)

*Requested Contribution from Psi-k (In EUROS)

*Primary Psi-k Working Group (choose only one)

- 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
- 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
- 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

Secondary Psi-k Working Group(s) (choose all that apply)

- 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
- 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
- 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

*Brief Abstract and Objectives for Event. This is the key component of the preproposal - from half a page to a full page.

*Provisional List of Proposed Speakers / Participants (no need to be confirmed).

If your workshop is part of a series (annual, biennial etc) please provide details of the series (dates, duration, location of last edition, number of participants and sources of funding) and explain how this edition differs from previous events

*Due to restrictions encountered as a result of covid-19 we are encouraging activities that highlight new approaches to research, teaching, and dissemination – feel free to propose novel and original ways, or digital remote versions of traditional events. Psi-k will consider funding equipment, software or subscription services that might be required, and will offer access to Zoom videoconferencing capabilities.

*Tentative Budget - as a guide requested Psi-k contributions are expected to be up to 30 EUROS per participant, per day.

Please indicate any additional sources of funding already secured or applied for (including the date when a decision is expected)

If you have extra information that you think will enhance your application you may upload a pdf file here. *Please note that you are only able to upload **ONE** file with your application and only pdf files will be accepted, so if you have multiple files you must merge them into one pdf document before uploading.*