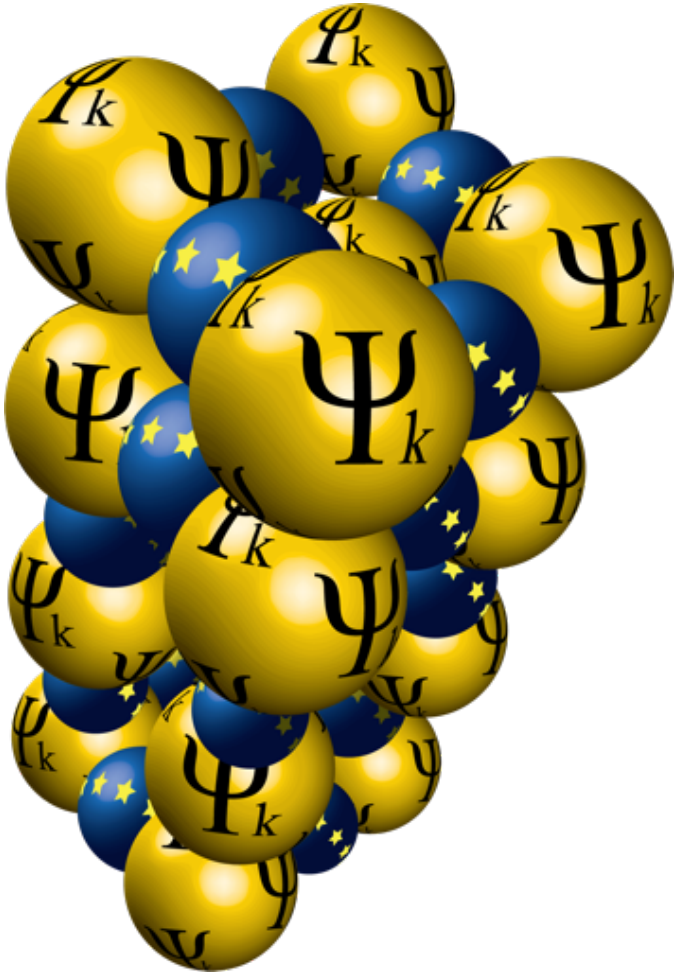
GENERAL PSI-K COMMUNITY MEETING

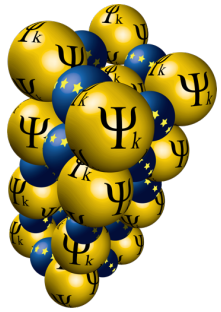
Fri Nov 27 2020, 2pm CET

http://psi-k.net



PSI-K MISSION

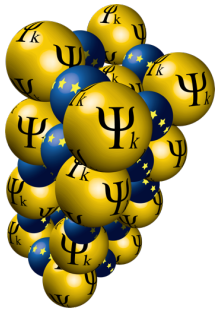
Psi-k is a Europe-based, worldwide network of researchers working on the advancement of first-principles computational materials science. Its mission is to develop fundamental theory, algorithms, and computer codes in order to understand, predict, and design materials properties and functions. Theoretical 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 organization of conferences, workshops, tutorials and training schools as well as the dissemination of scientific thinking in society.



HISTORY (AND PREHISTORY)

The idea of creating Psi-k came from CCP9, the UK's Computational Collaborative Project No 9, on the "Electronic Structure of Solids", funded through the UK's Science Research Council (SRC) in 1981. Volker Heine was instrumental in establishing CCP9, one of a number of computational collaborative projects (CCPs) funded at the time by SRC to support research at UK's universities. Balazs Gyorffy (Bristol) became the first, long term, CCP9 chairman, and Walter Temmerman (Bristol, Daresbury Laboratory), its scientific secretary.

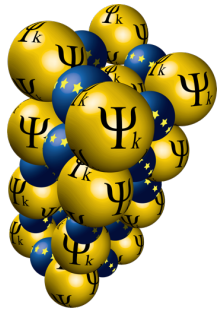
The greatest opportunity presented itself with the European Union's Human Capital and Mobility (HCM) Framework III Programme (FP3). A proposal application to FP3, prepared by Volker Heine, and Walter Temmerman, to create a network of European researchers in the field of "Ab-initio (from first-principles) electronic structure calculations of complex processes in materials", was successful and granted three-year funding of in total 400k EUR, from 1994 to 1996.



https://www.scd.stfc.ac.uk/Pages/The-story-of-Psi-k.aspx

Z. (Dzidka) Szotek, Leon Petit, Paul Durham

VOLKER HEINE, WALTER TEMMERMANN, ZDIZKA SZOTEK



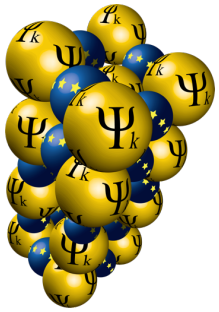
THE FIRST GENERAL PSI-K CONFERENCE (1996)

Network Conference

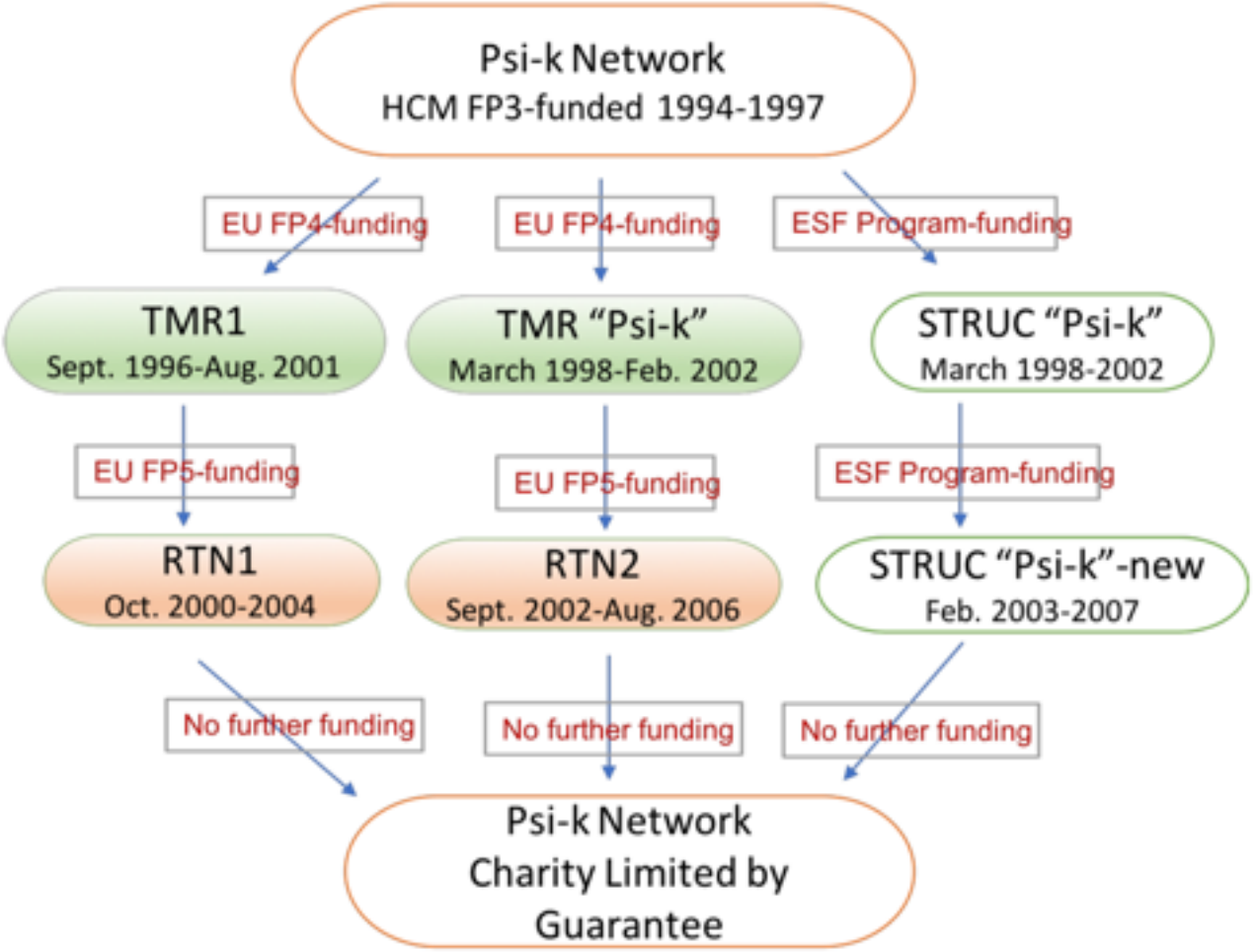
organized by the European Union HCM network

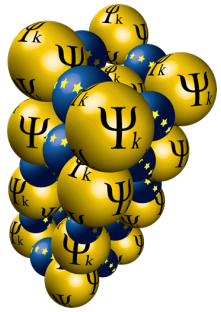
"Ab initio (from electronic structure)
calculation of complex processes
in materials"

Schwäbisch Gmünd, Germany
September 17-21, 1996



MOVING ON


Psi-k Network
HCM FP3-funded 1994-1997
EU FP4-funding
EU FP4-funding
ESF Program-funding
TMR1
Sept. 1996-Aug. 2001
TMR "Psi-k"
March 1998-Feb. 2002
STRUC "Psi-k"
March 1998-2002
EU FP5-funding
EU FP5-funding
ESF Program-funding
RTN1
Oct. 2000-2004
RTN2
Sept. 2002-Aug. 2006
STRUC "Psi-k"-new
Feb. 2003-2007
No further funding
No further funding
No further funding
Psi-k Network
Charity Limited by
Guarantee



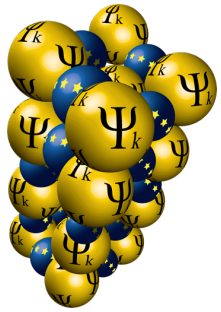
PETER DEDERICHS, RISTO NIEMINEN, DAMIAN JONES

PSI-K ACTIVITIES

- Workshops, tutorials, schools, code retreats: 25-30 every year
  http://psi-k.net/workshops/

- CECAM-Psi-k Research Conference: 1 every year
  https://psi-k.net/cecam-psi-k-research-conferences/

- Psi-k General Conference: every 5 years
  https://www.psik2020.net/home

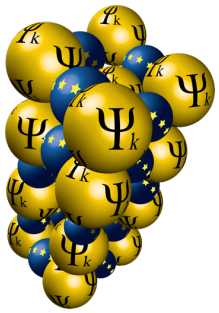


PSI-K DISSEMINATION

- Web site: https://psi-k.net/

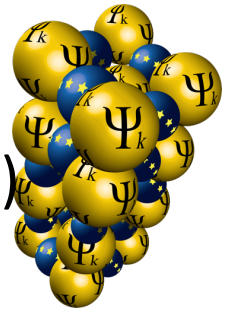
- Mailing list – 6000+ recipients. Everyone can post Events, Job ads, General announcements (with care and moderation) https://psi-k.net/mailing-list/

- Psi-k highlights – can be also submitted to IOP Electronic Structure and npj Computational Materials (contact leon.petit@stfc.ac.uk) https://psi-k.net/highlights/



PSI-K ORGANIZATION

- Chair and Trustees (UK Charity law)
- Scientific Advisory Council – 82 members, meets once a year in November to discuss and approve activities http://psi-k.net/scientific-advisory-committee/
- Working Groups: 16 groups of 5 scientists each, in the 3 domain coordinated by a Trustee
  - Physical formalisms (S. Biermann)
  - Algorithms, software, and data (A. Mostofi)
  - Applications to real materials and materials design (I. Abrikosov)



A: Physical formalisms – Silke Biermann

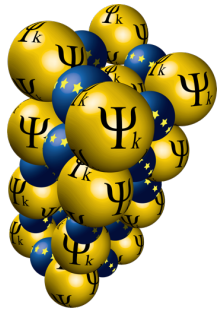
A1. Density and density-matrix functional theories – Miguel Marques *including improved functionals and time-dependent DFT*

A2. Perturbative many-body methods – Georg Kresse & Lucia Reining *including RPA, ACFDT, GW, Bethe-Salpeter and coupled cluster methods*

A3. Non-perturbative many-body methods – Massimo Capone, Jan Kunes & Michele Casula *including DMFT and Quantum Monte Carlo methods (VMC, DMC, FCI-QMC etc)*

A4. Open and non-equilibrium systems – Sara Bonella & Stefan Kurth *including transport*

A5. Quasi-particle interactions and spectroscopies – Claudia Draxl & Lilia Boeri *including coupling of electrons and spins to external fields, magnons, phonons, polarons and addressing phenomena such as superconductivity*



B: Algorithms, software and data – Arash Mostofi

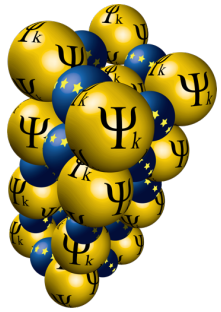
B1. Reduced-scaling methods – Javier Junquera *i.e. reduced scaling of computational effort with system-size*

B2. Statistics and configuration sampling – Michele Ceriotti *including* ab initio *thermodynamics, molecular dynamics, structure searching & cluster expansion*

B3. Bridging length- and time-scales – Karsten Reuter *including metadynamics, transition path search & sampling, modelling of kinetics and embedding*

B4. Software engineering – Xavier Gonze & Micael Oliveira *including high performance computing and shared libraries*

B5. High-throughput screening and data analytics – Luca Ghiringhelli & Geoffroy Hautier *including computational materials discovery, database mining and machine learning*



C: Applications to real materials and materials design – Igor Abrikosov

C1. Structural materials – Jörg Neugebauer *including metallic alloys, minerals, amorphous solids and materials under extreme conditions*

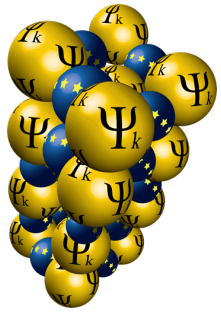
C2. Functional materials and devices – *including energy materials*

C3. Magnetism and spintronics – Ingrid Mertig & Silvia Picozzi *including multiferroics and topological materials*

C4. Surfaces and interfaces – Axel Groß & Sergey Levchenko *including catalysis and electrochemistry*

C5. Nanoscale structures (2D, 1D, 0D) and related phenomena – Kristian Thygesen

C6. Molecules, macromolecules and biomolecules – Carla Molteni



TRUSTEES


Igor Abrikosov


Silke Biermann

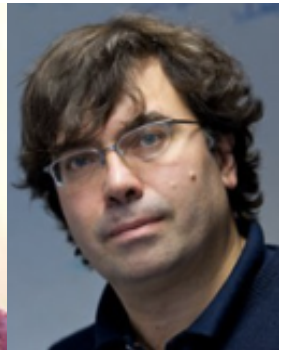

Stefan Bluegel


Peter Dederichs


Claudia Draxl


Peter Haynes


Volker Heine


Nicola Marzari


Elisa Molinari


Arash Mostofi


Risto Nieminen


Mike Payne


Lucia Reining


Angel Rubio

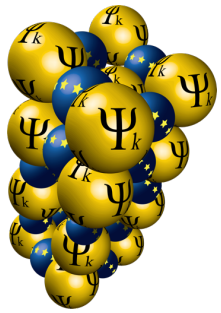

Matthias Scheffler

NEW CHAIR: PETER HAYNES (IMPERIAL COLLEGE)

HOW CAN YOU CONTRIBUTE?

- Funding: we are a charity, and we rely on donations from goodwill parties – currently receiving ~150,000 eur/year. Contact damian.jones@stfc.ac.uk

- Participate! Submit proposals (instructions on website), become part of a working group (contact working group leaders), suggest a new one (contact the domain coordinator)



https://www.psik2020.net/

THANKS!

AND QUESTIONS, IN THE CHAT