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For the latest information on this
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EUROPEAN SCIENCE FOUNDATION
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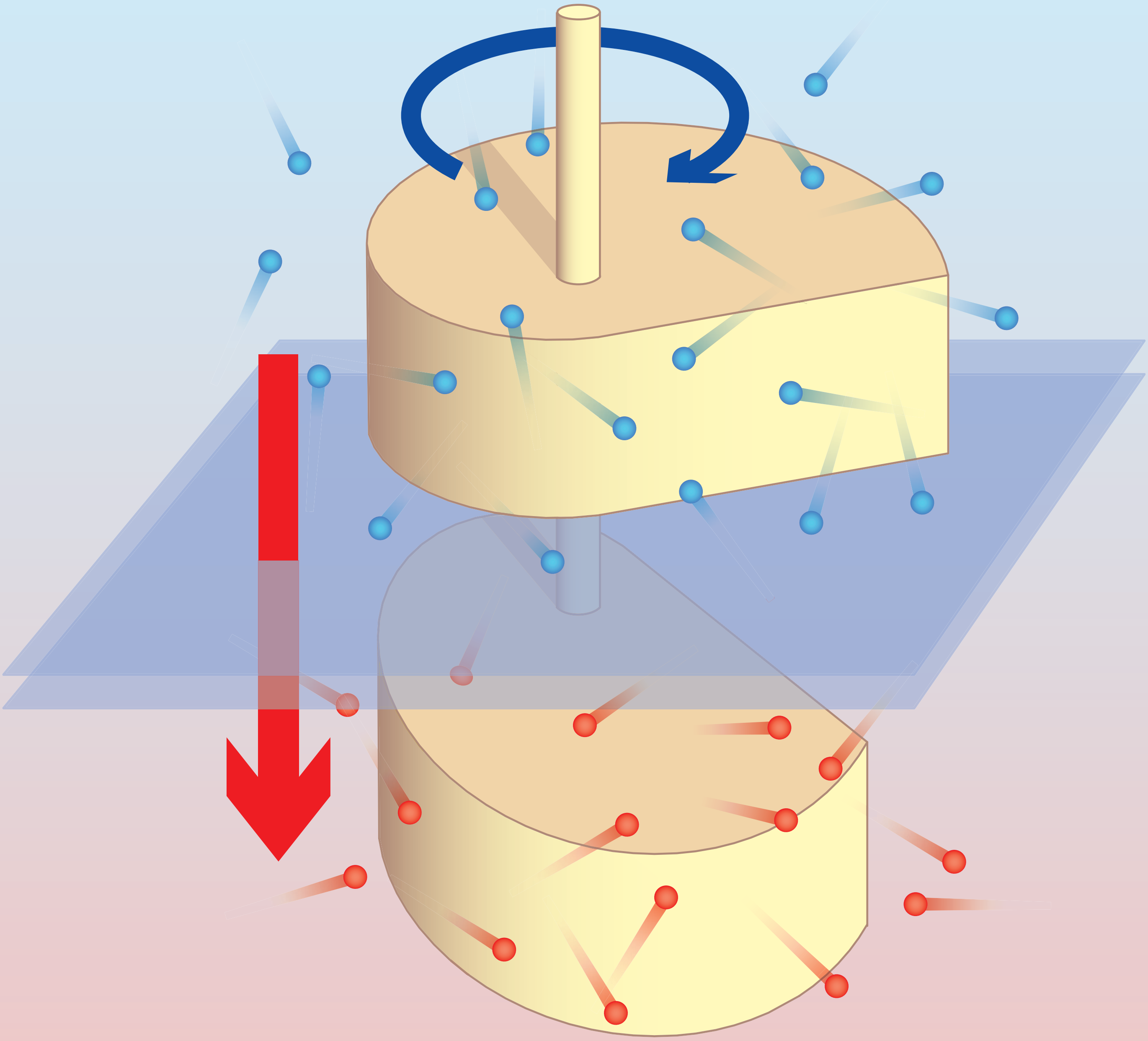
RESEARCH NETWORKING PROGRAMME

EXPLORING THE PHYSICS OF SMALL DEVICES (EPSD)

Standing Committee for Physical and Engineering Sciences (PESC)



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Introduction

The European Science Foundation (ESF) is an independent, non-governmental organisation, the members of which are 80 national funding agencies, research-performing agencies, academies and learned societies from 30 countries.
The strength of ESF lies in the influential membership and in its ability to bring together the different domains of European science in order to meet the challenges of the future.
Since its establishment in 1974, ESF, which has its headquarters in Strasbourg with offices in Brussels and Ostend, has assembled a host of organisations that span all disciplines of science, to create a common platform for cross-border cooperation in Europe.
ESF is dedicated to promote collaboration in scientific research, funding of research and science policy across Europe. Through its activities and instruments ESF has made major contributions to science in a global context. The ESF covers the following scientific domains:

- **Humanities**
- **Life, Earth and Environmental Sciences**
- **Medical Sciences**
- **Physical and Engineering Sciences**
- **Social Sciences**
- **Marine Sciences**
- **Nuclear Physics**
- **Polar Sciences**
- **Radio Astronomy Frequencies**
- **Space Sciences**

Recent technical, experimental, conceptual and theoretical advances have opened new perspectives, not only for the study or understanding of small systems, but also for their manipulation, control and manufacture. The theoretical breakthroughs offer a new vision of the relationship between the micro and macro worlds, in particular the impact of dynamical randomness, the relationship between fluctuations, entropy production and work, and the role of stochasticity in small-scale non-linear non-equilibrium phenomena. On the conceptual side, rather than miniaturising the construction and principles of macroscopic machines, one can build on the specificities of the small scale, such as the presence of a strong stochastic component, to propose new designs and new modes of operation. Advances in the study, measurement, manipulation or even manufacture of small devices are even more spectacular. The technical and experimental breakthroughs include a whole array of new measuring, manufacturing and controlling devices such as atomic force microscopy, scanning probe microscopy, field emission microscopy, optical tweezers, an array of techniques from lithography, biotechnology and supra-molecular chemistry, and many new and improved methods developed in nanotechnology (nanoelectronics, nanomedicine, nanotubes, microfluids).

Our Network offers a unique expertise spanning the whole range from purely theoretical research to experimental and applied research. The majority of the laboratories are in fact involved in experimental research, while the theoretical groups are at the forefront of recent developments concerning the physics of small devices. Topics include: non-equilibrium statistical mechanics, stochastic processes, stochastic thermodynamics, non-linear dynamics, numerical techniques, control theory, pattern formation, nanoelectronics and nanomaterials, charge transport and thermal properties in nano and microstructures, biotechnology of small devices, catalysis at the nanoscale, experimental and theoretical biophysics of the cell, new computation techniques for free-energy estimation, Brownian refrigerator in nanosuperconductors, issues of Carnot efficiency for Brownian motors, various proposals for microsieves and other microfluidic devices.

The running period of the ESF EPSD Research Networking Programme is five years from March 2009 to March 2014.

Cover picture:
A Brownian refrigerator pumps heat from a cold to a hot reservoir by exerting a torque on asymmetric objects (Courtesy of C. Van den Broeck).

Aims and Objectives

EPSD brings together leading European laboratories at the forefront of experimental studies of small physical and biophysical devices with theoretical groups that have pioneered recent spectacular advances in the non-equilibrium physics of small systems. Such a unique cross-disciplinary Network will push forward the integration between theory, experiment and application, allowing the resolution of technical problems specific to the small scale, and inspire new methods of design, manipulation and operation. The aim of EPSD is to further develop and apply the thermodynamics and statistical mechanics of small non-equilibrium devices, evaluate the role of stochasticity and non-linearity, implement optimisation techniques and develop new analytical approaches for small driven systems. Important inspiration will also be drawn from the incorporation of groups working on the physical understanding of biological machines, such as molecular motors and other 'devices' operating in the cell, and their corresponding biotechnological applications. The implications of these new theoretical and conceptual perspectives will be confronted with practical and technological issues posed by the design and construction of small-scale devices, in synergy with the participating research laboratories working on nanoelectronics, nanorefrigeration, supramolecular devices, catalytic devices, biotechnology of the cell, microfluidics and micro-arrays. The Programme will also devote special attention to the training of young scientists in order to broaden their expertise.

Topic Areas

a) Theoretical concepts

Since the 1990s several European groups have recorded major advances in the theoretical and conceptual description of small systems. One class of results is related to what is usually referred to as 'fluctuation and work theorems'. These results extend the pioneering work of Onsager to far from equilibrium situations. They can be derived at the Hamiltonian level and provide a new foundation for the Second Law of Thermodynamics and the interpretation of irreversibility, and can also be formulated more generally for dynamical systems.

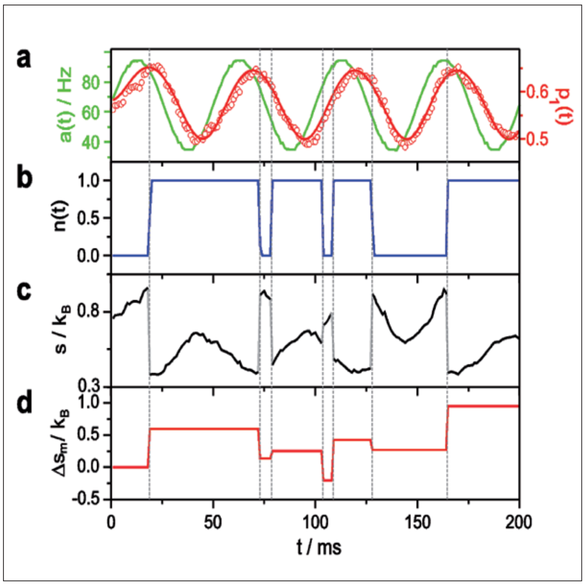

Figure 1. Entropy production in an optically driven defect centre in diamond, modelled as a two-level system: (a) transition rate (green line) and probability of the bright state (red line); (b) a single trajectory; (c) evolution of the system entropy and entropy change of the medium for that specific trajectory, as given by stochastic thermodynamics (Courtesy of U. Seifert).

When operating on the mesoscopic scale, relevant for some physical and chemical and most biophysical applications, a new field called 'stochastic thermodynamics' or 'path thermodynamics' has been developed. This approach generalises the classical concepts of thermodynamics to small-driven systems by assigning a stochastic entropy and a weight to each phase-space path. Exact results for the distribution of work and entropy production can be derived. In some cases, dynamical phase transitions may occur which are associated with exponential tails in the work or entropy flow distributions. Since successful comparisons with experimental model systems have proved the fundamental potency of this new framework, it can and should now be applied to both more complex biological systems and technologically relevant devices.

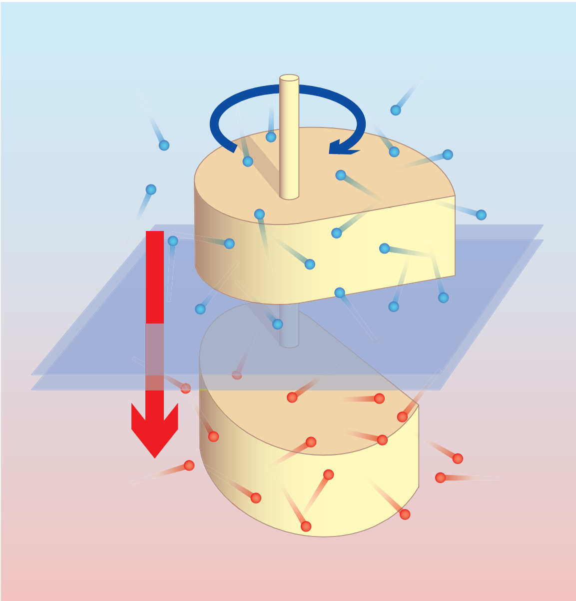

Figure 2. A Brownian refrigerator pumps heat from a cold to a hot reservoir by exerting a torque on asymmetric objects (Courtesy of C. Van den Broeck).

The concept of thermodynamic stability and, in particular of a phase transition itself, has to be revisited when dealing with small systems. When discussing structural and morphological phase transitions in nanoparticles, one has to realise that the physical and chemical properties can change dramatically essentially due to the large surface-to-volume ratio. Transformation pathways blocked in the macroscopic material might become favoured in the nanoparticle, because they lead to shapes with particularly low surface free energies. Also, thermal fluctuations, which affect the stability of nanoparticles, are of increasing importance as size is scaled down. In view of the possible use of such nanoscale systems as building blocks for novel devices, understanding these effects on an atomistic level is of fundamental importance.

b) Physical devices

The appearance of fluctuations in small systems has led to new concepts for characterising or operating such devices, exploiting rather than fighting these very same fluctuations. We cite the principles of Brownian motors, stochastic resonance and resonant activation, Brownian refrigerator, stochastic synchronisation, Parrondo paradox and free-energy estimations from fluctuations. The basic question about the efficiency of such devices has to be re-examined. For operation far from equilibrium, one can wonder whether the efficiencies predicted close

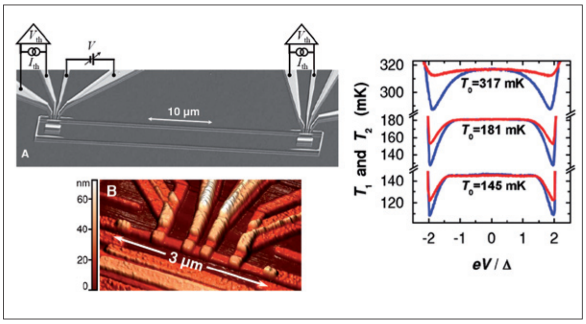

Figure 3. Cooling at the quantum limit. Electronic refrigerators operate at very low temperatures, reaching a temperature of few tens of millikelvin. Top left: the sample with two resistors separated by a distance of 50 micrometres enclosed in a superconducting loop. Bottom left: a close-up of one of the normal metal resistors with attached electrodes. Right: experimental data of NIS electronic cooling of the island directly connected to the refrigerator (blue line) and of the remote island (red line). Remote cooling persists down to the lowest temperatures indicating electromagnetic energy exchange between the resistors."
(Courtesy of J. Pekola)

to thermodynamic equilibrium, such as the Carnot and Curzon-Ahlborn efficiency, can be reached. In particular it appears that very high efficiencies are attained in biological motors. The understanding of these mechanisms from the new theoretical perspectives has obviously great technological potential. Besides the direct application to thermally, optically or chemically driven nanomotors, these insights can guide the design for nanoversions of the refrigerator, the thermo-couple, the Peltier element and the photovoltaic cell.

Concerning electro-thermal or electro-optical processes, we note the charge transport and thermal

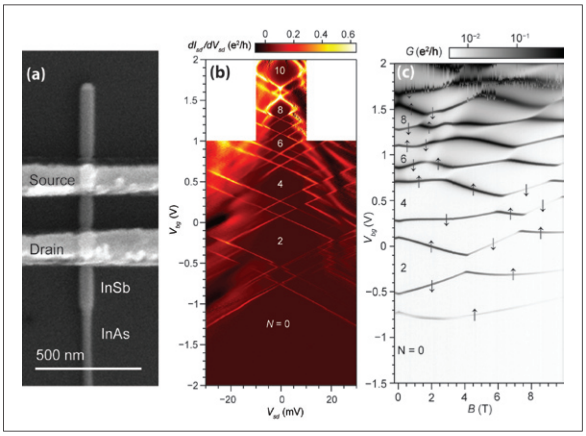

Figure 4. (a) SEM image of an InSb nanowire quantum dot device. (b) Charge stability diagram measurements of the dot, where few-electron Coulomb blockade effect and the Kondo effect are clearly observed. (c) Evolution of the conductance peaks in a small bias regime with an increasing the magnetic field (Courtesy of H. Xu).

properties in nano and microstructures. The interplay of the various relaxation rates and the energy filtering of electrons in superconducting metal structures opens a very versatile and well controlled domain for studies of thermal phenomena in nanosized structures and devices. These include quantised thermal conductance by photons, cyclic electronic refrigeration using a single-electron charging effect and energy filtering, and Brownian refrigeration of electrons.

The interplay between fluctuations, disorder and collective phenomena can also be observed in micro and nanostructured materials fabricated by means of lithographic techniques. A rich phenomenology of ratchet effects has been observed for fluxons in superconducting films and also in the motion of domain walls in magnetic materials, providing new design strategies for nanodevices.

Small devices can easily be driven into the strong non-linear response regime where they exhibit novel electrical properties. An example of these is a three-terminal ballistic junction device, which can be used as a non-linear signal rectifier and the building block for novel logic circuits. Another example is the double quantum dot device which, in view of the double-well potential for electrons, can be employed as a stochastic resonance device. Such an enhancement of weak input signals can also be demonstrated using semiconductor heterostructures, with particular interest regarding the sensitivity limit in the single-electron operation regime.

The existing devices based on compound semiconductor quantum wells, wires and dots require a deeper understanding of properties of their electronic states, dynamic behaviour and other physical properties in the quantum nanostructures. Potential future semiconductor nanodevices, such as spinotronic or those based on quantum wires, need to be studied from the fundamental scientific point of view.

c) Biochemical devices

Some of the recent advances of synthetic chemistry also require a theoretical framework based on the physics of small systems. Chemists have demonstrated imagination and considerable skill in the design and construction of synthetic molecular systems in which positional displacements of submolecular components result from moving downhill in terms of energy. But what are the structural features necessary for molecules, which are undergoing incessant Brownian motion, to repetitively do mechanical work? How can we make a molecular machine that pumps ions to reverse a concentration gradient, for example, or moves itself uphill in terms of energy? How can we make nanoscale structures that traverse a predefined path across a surface or down a track by responding to the nature of their environment so as to change direction? How can we make a synthetic molecular motor that rotates against an applied torque?

Artificial compounds that can do such things have yet to be realised. However, the fundamental guidelines necessary to invent them are being studied by physicists. A close interaction between chemists and physicist is needed to understand how these often theoretical ideas can be implemented into actual synthetic molecular structures to create working experimental artificial molecular machines. The Network will promote such collaboration to explore the possibility of producing experimental examples of some or all of the following types of mechanism: flashing ratchets, tilting ratchets, Seebeck ratchets, drift ratchets, Hamiltonian ratchets, temperature ratchets and entropic ratchets.

Catalysis is another immensely important field of research, for which the understanding of the interplay between physics and chemistry on the very small scale is essential. In field emission microscopy, atoms at the tip are ionised by a high electric voltage, allowing the observation of crystal facets and their dynamics on the nanoscale. This technique is used to study chemical reactions of heterogeneous catalysis with nanometric resolution. In particular, oscillating chemical reactions have been observed in the reduction of NO_2 with H_2 on platinum or in the O_2 + H_2 reaction forming water on rhodium. These systems are typical out-of-equilibrium nanosystems. The understanding of these processes at the nanoscale remains an open problem, with obvious technological implications for the construction of catalytic devices.

d) Optimisation

The description of small-scale non-equilibrium systems by stochastic thermodynamics provides natural criteria to optimise the form of the driver; i.e. the external protocol. An obvious cost function for such an optimisation is the mean dissipated work spent in a finite-time process. The recent analysis of simple model systems has shown that even for apparently trivial systems with given initial and final states, the optimal protocol shows intricate features such as singularities at the beginning and the end of the process. This insight will also become relevant for the efficient computational determination of free-energy differences using the Jarzynski relation. Furthermore, optimisation with respect to maximum power in thermal machines has also revealed features of universality, deriving from underlying microreversibility. It is clearly of great interest to address similar questions in the context of chemical engines.

From a more engineering point of view, we note that there is a great interest from transport industries for optimisation in tiny parts production and assembly processes. In the highly customised world of manufacturing and assembly lines, non-equilibrium statistical mechanics and thermodynamics offers the suitable unifying framework needed to develop general operating principles and optimisation methods. Conceived to operate far from thermodynamic equilibrium, production systems sustain flows of matter, energy and information which ultimately transform raw material to structured finished goods. In micrometric ranges and even below, the production of devices formed by microparts raises original challenges belonging to the core objective of the Network. To manufacture and assemble microdevices, one needs to stir, sort, orient, wrap, screw and transport. All these elementary manufacturing operations are ruled by mesoscale physics laws.

e) Fluid transport

Water in confined geometries has properties that can dramatically differ from those of bulk water. For instance inside narrow pores with a subnanometer diameter, water forms single-file chains of hydrogen-bonded molecules that are orientationally ordered over long distances. Interestingly, the remarkable properties of nanopore water are captured by simple dipole lattice models that can be studied very efficiently using computer simulations as well as in complex geometries. One-dimensional water wires are of essential importance for many biological processes, such as water and proton transport through cell membranes, and may be harnessed in future membrane materials for use in hydrogen fuel cells and sensing devices.

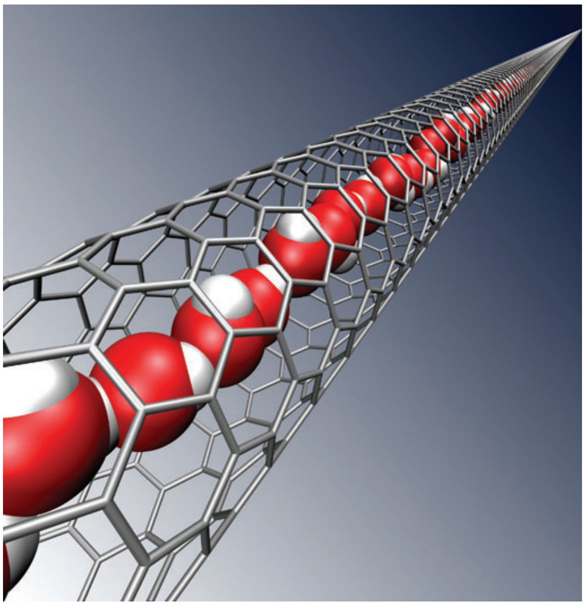

Figure 5. Chains of water molecules inside a nanopore (Courtesy of C. Dellago).

An understanding of flow in porous media is central to progress in such diverse fields as petroleum extraction, pollutant transport in the ground and blood transport in tissue. When there is more than one fluid competing for space and transport in the porous medium and these fluids do not mix, the ensuing flow properties become exceedingly complex. Even though flow in porous media has a history stretching back decades, there are large areas of knowledge yet to explore. This has important implications. For example, 20 to 60% of the oil remains in a typical oil reservoir at the point it is declared economically unviable and abandoned.

Our work on transport in porous media concerns the steady-state flow of immiscible fluids. Assuming there are two fluids, one of them will dominate and the other will form clusters that merge and split up, but in such a way that all macroscopic parameters describing the flow fluctuate around fixed averages. The steady state is the typical situation encountered in porous media flow, rather than transient flow. However, whereas the latter has been studied extensively over the last decades, little has been done in connection with the former.

One of the main goals for this work is to be able to provide computational methods that provide predictive power on a scale that at present is lacking in porous media flow engineering. This may in turn prolong the period in which the world can continue its overwhelming dependence on oil as an energy source so that other technologies will have time to reach maturity before they become indispensable.

EPSD Activities

EPSD promotes collaboration among groups working on these topics by funding workshops, schools and conferences, as well as exchange visits of scientists and graduate students.

Workshops and schools

The Programme envisages the organisation of one main event (school or conference) every one or two years, and the funding of 5 to 10 small thematic or exploratory workshops per year.

Applications for science meetings should be submitted online on the ESF EPSD website, during September and October of the year previous to the event. The precise deadline for applications will be announced on the website.

Short visits and exchange grants

EPSD supports collaborations among groups in the field by short visit grants, for periods of up to 14 days, and research grants covering stays between two weeks to six months. Applications can be submitted online on the ESF EPSD website, and they will be received on a running basis.

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