Symposium Frontiers of Electronic Structure Theory: Discovery of Novel Functional Materials (SYES)

jointly organized by
the Surface Science Division (O),
the Thin Films Division (DS),
the Semiconductor Physics Division (HL),
the Magnetism Division (MA),
the Metal and Materials Physics Division (MM), and
the Low Temperature Physics Division (TT)

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The predictive accuracy that quantum-mechanical simulations have now reached for realistic, complex systems opens the possibility of using them as a systematic tool for the discovery and design of new materials, accelerating and streamlining the development of novel solutions to technological problems, and overcoming traditional approaches based on empirical rules, as the talks in this symposium will demonstrate.

Overview of Invited Talks and Sessions

(Lecture Room H1)

Invited Talks

SYES 1.1	Fri	9:30–10:00	H1	**Molecular dynamics simulation of nucleation and growth of crystals from solution** — •Michele Parrinello
SYES 1.2	Fri	10:00–10:30	H1	**Describing, understanding, and discovering hybrid materials from first principles** — •Claudia Draxl
SYES 1.3	Fri	10:30–11:00	H1	**Mapping the Electronic Structure Landscape for Materials Discovery** — •Krishna Rajan
SYES 1.4	Fri	11:00–11:30	H1	**New ferroelectrics and antiferroelectrics by design** — •Karin Rabe
SYES 1.5	Fri	11:30–12:00	H1	**The Materials Project: The design of materials using high-throughput ab initio computations** — •Gerbrand Ceder

Sessions

SYES 1.1–1.5	Fri	9:30–12:00	H1	**Symposium Frontiers of Electronic Structure Theory: Discovery of Novel Functional Materials (SYES)**

SYES 1: Symposium Frontiers of Electronic Structure Theory: Discovery of Novel Functional Materials (SYES)

Time: Friday 9:30–12:00 Location: H1

Invited Talk SYES 1.1 Fri 9:30 H1

Molecular dynamics simulation of nucleation and growth of crystals from solution — •Michele Parrinello — Department of Chemistry and Applied Biosciences, ETH Zurich and Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera Italiana, Lugano, Switzerland

Nucleation and growth of crystals from solution is a phenomenon of great practical relevance. Yet its study is rather challenging both experimentally and theoretically. Computer simulations could be of great help however they are rather difficult. To this effect we have developed a number of methods that can help overcoming many of the difficulties. We shall present results on the growth of urea from aqueous solutions in the presence and the absence of additives. We show how additives in particular biuret can control the shape of the growing crystal. We also show how the nucleation from saturated water solution of the humble NaCl hides some remarkable surprises.

Invited Talk SYES 1.2 Fri 10:00 H1

Describing, understanding, and discovering hybrid materials from first principles — •Claudia Draxl — Humboldt-Universität zu Berlin, Berlin, Germany

Hybrid materials are most exciting as one can expect new properties arising at the interface, which are absent in either of the building blocks. At the same time, they represent challenging cases for electronic-structure theory. Methods that turned out useful for describing one side may not be applicable for the other one, and they are likely to fail for the interfaces. For selected examples of organic/inorganic hybrid interfaces for light emitting applications and photovoltaics, I will present structural properties, electronic bands, and optical excitation spectra as obtained from density-functional theory and many-body perturbation theory. They will highlight which properties can be reliably computed for such materials. It needs to be also discussed, however, what is missing to reach predictive power on a quantitative level and, thus, open a perspective towards the discovery of new materials.

Invited Talk SYES 1.3 Fri 10:30 H1

Mapping the Electronic Structure Landscape for Materials Discovery — •Krishna Rajan — Iowa State University, Ames IA, USA

Normally, structure*property relationships are guided by defined functional relationships (e.g. electronic structure calculations to define energy landscapes associated with crystal chemistry) and many groups have developed powerful and extensive computational strategies based on electronic structure calculations to search large virtual chemical spaces to identify potentially new compounds. However, we propose a different approach to establish such a structure* property relationships where we do not assume any specific formulation linking structure with property. Rather, we take a data-driven approach where we seek to establish structure*property relationships by identifying patterns in a large and diverse array of data associated with both crystallographic and electronic structure calculations. By coupling statistical learning methods to map such high dimensional data in lower dimensions, we show how we can discover new materials chemistries with targeted properties.

Invited Talk SYES 1.4 Fri 11:00 H1

New ferroelectrics and antiferroelectrics by design — •Karin Rabe — Rutgers, the State University of New Jersey, USA

I will describe our work on the design and discovery of new classes of ferroelectric and antiferroelectric materials using a combined crystallographic database / first principles approach. For ferroelectrics, using the design principle that any polar structure type can have ferroelectric representatives if the barrier to switching is lowered by appropriate chemical variation, we have recently identified a new family of ferroelectrics in the intermetallic LiGaGe structure type. For antiferroelectrics, we used a design principle based on the close relationship between ferroelectrics and antiferroelectrics to identify a previously unrecognized class of antiferroelectrics, related to the LiGaGe-type ferroelectrics, in the MgSrSi structure type. The discovery of new classes of antiferroelectrics is expected to open the way to increased recognition and application of antiferroelectrics as functional materials.

Invited Talk SYES 1.5 Fri 11:30 H1

The Materials Project: The design of materials using high-throughput ab initio computations — •Gerbrand Ceder — Massachusetts Institute of Technology, Cambridge MA, USA

The need for novel materials is the technological Achilles Heel of our strategy to address the energy problem facing the world. The "Materials (Genome) Project*, has as its objective to use high-throughput first principles computations on an unparalleled scale to discover new materials for energy technologies. Only computationally driven materials design can deal with the scale and urgency of the materials discovery problem. I will show how several key problems such as crystal structure prediction and accuracy limitations of standard Density Functional Theory methods have been overcome to perform reliable, large scale materials searching. In addition, once large data sets are developed, machine learning can be used to extract insight and design rules. I will show successful examples of high-throughput calculations in the field of lithium batteries, and show several new materials that have been discovered. In addition, I will discuss the public release version of the Materials Project which is making large quantities of computed data freely available to the materials community. (www.materialsproject.org).