SYID 1: Information Driven Materials Research

Time: Monday 9:30–12:00 Location: H 0105

Invited Talk SYID 1.1 Mon 9:30 H 0105

Data driven R&D for Materials: Cognitive Discovery — •Alessandro Curioni — IBM Research, Zurich ,Switzerland

Innovation in many key industrial sectors is demanding new materials with lower manufacturing costs, improved performance, and a reduced environmental footprint.

Decades of deep experimental as well as computational research for the discovery of novel materials have been creating vast amounts of data and supporting information. Indeed, hundreds of thousands of related papers and patents are published every year nowadays, while academic institutions and the Industry create Petabytes of crucial data by means of high fidelity materials simulations. Thus, a new opportunity arises today: extract the available knowledge from the literature, curate and connect it with the simulation structured data and therefore create a positive feedback loop that can dramatically accelerate the pace of discovery.

Of course there are several challenges in this quest. However, recent advances in Data Science and Machine Learning offer a very promising way forward. In this talk, I will describe this new approach, that we call Cognitive Discovery. We harness the power of Machine Learning, Natural Language Processing and novel knowledge representation and analysis methods to extract and curate knowledge and create data driven models. I will discuss applications of Cognitive Discovery in materials research and show its wider applicability in technical R&D.

Invited Talk SYID 1.2 Mon 10:00 H 0105

Rational design and synthesis of Pt-based catalysts for fuel cell applications — •Younan Xia — Department of Biomedical Engineering, Georgia Institute of Technology, Atlanta, GA 30332, USA

Platinum (Pt) is by far the best catalyst for a range of industrially important reactions, including the oxygen reduction reaction (ORR) involved in the operation of proton exchange membrane fuel cells (PEMFCs). Its low abundance, limited supply, and ever-increasing price have kept motivating researchers to minimize the loading of this precious metal in the catalyst. In this talk, I will discuss a number of strategies involving computational design and rational synthesis for greatly increasing the activity and durability of Pt-based ORR catalysts, including electronic coupling through alloying, surface strain engineering, facet-controlled synthesis, and increase of dispersion by switching to a core-shell or hollow structure. The same strategies can also be applied to other precious metals such as ruthenium (Ru), rhodium (Rh), and iridium (Ir) to significantly reduce their loadings in catalysts without compromising their performance. These strategies will enable us to achieve a sustainable use of precious metals in energy conversion, industrial catalysis, and other related applications.

Invited Talk SYID 1.3 Mon 10:30 H 0105

2D, or not 2D? Materials discovery, data provenance, and workflow reproducibility. — •Nicola Marzari — MARVEL NCCR, EPFL, Lausanne, Switzerland

Two-dimensional materials have seen in the past decade very dedicated experimental and theoretical efforts in the quest for novel physics and functionalities. Here, we systematically explore with first-principles calculations known inorganic materials, to identify those that could be exfoliated into two-dimensional layers. We start by curating experimental materials databases, collecting reliable data for 110,000 unique compounds. Then, we identify those that appear layered according to simple geometric and bonding criteria, and launch high-throughput calculations - based on van-der-Waals density-functional theory and 2D density-functional perturbation theory - to characterize binding energies, stability, and properties. Remarkably, we find close to 2000 inorganic compounds that could be exfoliated into novel two-dimensional materials, and recover in the process the known ones - from graphene to transition-metal dichalcogenides to boron nitride and black phosphorus. I'll provide a perspective on the promising properties we are uncovering - topological, electrical, magnetic, chemical - while highlighting the need for scalable approaches to data and calculations, able to persist and query the full provenance of the data and ensure reproducibility of the calculations' workflows.

Invited Talk SYID 1.4 Mon 11:00 H 0105

Generating and assessing data from combinatorial and high-throughput experiments for the design of new materials — •Alfred Ludwig — Institute for Materials, Ruhr-University Bochum,44780 Bochum, Germany — ZGH and MRD, Ruhr-University Bochum,44780 Bochum, Germany

Design of new materials is a key challenge in materials science: e.g. new materials for future energy systems are urgently needed. Thin film combinatorial materials science (CMS) enables an efficient generation of consistent and large datasets on (unexplored) multinary materials, promoting the discovery and optimization of new materials. CMS can also rapidly verify or falsify theoretical or computational materials predictions. CMS comprises fabrication and processing of thin film materials libraries by combinatorial sputter deposition and processing, followed by extensive high-throughput characterization of the thin film samples contained in the libraries. The large datasets which are produced by the combinatorial approach need to be analyzed with new software tools, e.g. for the rapid assessment of X-ray diffractograms, necessary for the mapping of phase diagrams. Obtained results for ternary and quaternary systems are visualized in the form of composition-processing-structure-function diagrams, interlinking compositional data with structural and functional properties. The talk will cover and discuss examples of the combinatorial development of intermetallic materials for shape memory alloys, superalloys and thermoelectric applications as well as the development of metal oxide thin film materials libraries for solar water splitting.

Invited Talk SYID 1.5 Mon 11:30 H 0105

Novel materials discovery: big-data-analytics methods and infrastructure for building maps of materials — •Luca Ghiringhelli — Fritz-Haber-Institut der MPG, Berlin

The number of possible materials is practically infinite, while only few hundred thousands of (inorganic) materials are known to exist and for few of them even basic properties are systematically known. In order to speed up the identification and design of new and novel optimal materials for a desired property or process, strategies for quick and well-guided exploration of the materials space are highly needed. A desirable strategy would be to start from a large body of experimental or theoretical data, and by means of "big-data-analytics" methods, to identify yet unseen patterns or structures in the data. This leads to the identification of maps (or charts) of materials where different regions correspond to materials with different properties. The main challenge on building such maps is to find the appropriate descriptive parameters (called descriptors) that define these regions of interest. Here, I will present methods for the machine-aided identification of descriptors and materials maps applied to the metal/insulator classification, the prediction of novel 2D topological insulators, and of CO_2 adsorption-energy and activation on metal-oxide surfaces. I will also describe the infrastructure to perform such analyses online, via the "Big-data-analytics toolkit" within the framework of the Novel-Materials-Discovery (NOMAD) Laboratory.