# Symposium Information Driven Materials Research (SYID)

jointly organized by
the Surface Science Division (O),
the Thin Films Division (DS),
the Semiconductor Physics Division (HL), and
the Metal and Material Physics Division (MM)

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Materials Research is increasingly driven by the demand for ever faster and more targeted development of new structural and intelligent functional materials and their associated customized manufacturing methods. In order to meet this challenge, novel information based approaches to materials development are intensely investigated. These novel strategies encompass, but are not limited to, data- and simulation-driven materials development. While these strategies offer exciting opportunities to improve existing or tailor radically new materials for a wide range of key applications, they also still face unique challenges. In data-driven research the so-called *4 V challenge* is becoming eminent: Volume (the amount of data), Variety (the heterogeneity of form and meaning of data), Velocity (the rate at which data may change or new data arrive), Veracity (uncertainty of quality). The last item has been identified as being of particular importance for the big-data issues in materials science. An additional key challenge and enormous chance lies in the exploitation of the information content in available materials data-sets, which requires new and dedicated technology based on approaches in statistical and machine learning, computer science, statistics and information technology. Regarding simulation based strategies the development of truly predictive multiscale methodologies to compute macroscopic materials properties on the basis of their microscale constituents remains an enormous challenge. A key component of this problem is the need to develop transferable and robust scale-bridging protocols in the absence of simulation methods that cover all relevant time- and length-scales.

## Overview of Invited Talks and Sessions
(Lecture room H 0105)

### Invited Talks

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| SYID 1.1 | Mon | 9:30–10:00 | H 0105 | **Data driven R&D for Materials: Cognitive Discovery —** •Alessandro Curioni |
| SYID 1.2 | Mon | 10:00–10:30 | H 0105 | **Rational design and synthesis of Pt-based catalysts for fuel cell applications —** •Younan Xia |
| SYID 1.3 | Mon | 10:30–11:00 | H 0105 | **2D, or not 2D? Materials discovery, data provenance, and workflow reproducibility. —** •Nicola Marzari |
| SYID 1.4 | Mon | 11:00–11:30 | H 0105 | **Generating and assessing data from combinatorial and high-throughput experiments for the design of new materials —** •Alfred Ludwig |
| SYID 1.5 | Mon | 11:30–12:00 | H 0105 | **Novel materials discovery: big-data-analytics methods and infrastructure for building maps of materials —** •Luca Ghiringhelli |

### Sessions

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| SYID 1.1–1.5 | Mon | 9:30–12:00 | H 0105 | **Information Driven Materials Research** |