

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)
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