

Symposium Modern developments in multiphysics materials simulations (SYMS)

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

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Overview of Invited Talks and Sessions

(lecture rooms A 053 and A 151; Poster F)

Invited Talks

SYMS 1.1	Thu	14:00–14:30	A 151	Valence-dependent analytic bond-order potentials for metals and semiconductors — •D.G. PETTIFOR, R. DRAUTZ, T. HAMMERSCHMIDT
SYMS 1.2	Thu	14:30–15:00	A 151	Modelling Fracture Processes: Macroscopic Consequences of Atomistic Details — P. GUMBSCH, J.R. KERMODE, T. ALBARET, D. SHERMAN, N. BERNSTEIN, M.C. PAYNE, G. CSÁNYI, •A. DE VITA
SYMS 1.3	Thu	15:00–15:30	A 151	Discovery of Novel Hydrogen Storage Materials: An Atomic Scale Computational Approach — •CHRIS WOLVERTON
SYMS 1.4	Thu	15:30–16:00	A 151	Phase-field simulation of microstructure evolution: Linking atomistics to processes and properties — •INGO STEINBACH
SYMS 1.5	Thu	16:00–16:30	A 151	QM/MM Studies of Biosystems — •WALTER THIEL
SYMS 1.6	Thu	16:30–17:00	A 151	Error-controlled multiscale modeling approaches to surface chemistry and catalysis — •KARSTEN REUTER

Sessions

SYMS 1.1–1.6	Thu	14:00–17:00	A 151	Modern developments in multiphysics materials simulations I
SYMS 2.1–2.8	Thu	18:30–19:30	Poster F	Modern developments in multiphysics materials simulations II - Poster (joined by SYEC posters)
SYMS 3.1–3.11	Fri	10:15–13:00	A 053	Modern developments in multiphysics materials simulations III