

Surface Science Division Fachverband Oberflächenphysik (O)

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Overview of Invited Talks and Sessions

(Lecture Rooms H15, H17, H31, H33, H36, H38, H42, and H45; Poster B1 and B2)

Invited Talks

O 1.1	Mon	9:30–10:15	H36	Exciton fission, quantum coherence, & solar energy conversion beyond the limit — ●XIAOYANG ZHU
O 12.1	Mon	15:00–15:45	H36	Interaction of Gas Phase Molecules with Nanostructured Model Supported Catalysts: Thermodynamics and Kinetics — ●SWETLANA SCHAUERMANN
O 25.1	Tue	9:30–10:15	H36	Flippable charge, magnetic, and orbital modulation at ferroelectric/manganite interfaces from first principles — ●SOHRAB ISMAIL-BEIGI
O 34.1	Tue	15:00–15:45	H36	Ultrafast Spin and Magnetization Dynamics and their Signatures in the Transient Band Structure — ●MARTIN WEINELT
O 37.1	Wed	9:30–10:15	H36	Single impurities in semiconductors studied by STM — ●PAUL KOENRAAD
O 48.1	Wed	15:00–15:45	H36	Surface-confined molecular nanoarchitectures: non-covalent and covalent construction and templated dynamics — ●FLORIAN KLAPPENBERGER
O 59.1	Thu	9:30–10:15	H36	Interatomic Potentials for Molecules, Solids, and Surfaces Based on Artificial Neural Networks — ●JÖRG BEHLER
O 69.1	Thu	15:00–15:45	H36	Electrocatalysis: from single crystals to single nanoparticles — ●MARC KOPER
O 82.1	Fri	9:30–10:15	H36	Plasmons, forces and currents in atomic and molecular contacts — ●RICHARD BERNDT
O 92.1	Fri	13:15–14:00	H36	Room-temperature electron spin filtering by ordered thin films of helical organic molecules — ●HELMUT ZACHARIAS

Topical Talks of the Focussed Session: Frontiers of electronic structure theory (jointly with HL and TT)

O 5.1	Mon	10:30–11:00	H36	Fully ab initio determination of free energies: Basis for high-throughput approaches in materials design — ●JOERG NEUGEBAUER, FRITZ KORMANN, MARTIN FRIAK, BLAZEJ GRABOWSKI, TIMANN HICKEL
O 28.1	Tue	10:30–11:00	H36	Materials for Alternative Energies: Computational Materials Discovery and Crystal Structure Prediction — ●CHRIS WOLVERTON
O 41.1	Wed	10:30–11:00	H36	Challenges in data-intensive computational materials design: methodology and infrastructure. — ●BORIS KOZINSKY
O 51.1	Wed	16:00–16:30	H36	Screening high throughput density functional theory calculations using simplified models. — ●GEORG K. H. MADSEN, INGO OPAHLE, ALESSANDRO PARMA, EUNAN J. MCENIRY, RALF DRAUTZ
O 62.1	Thu	10:30–11:00	H36	Atomic-scale design of energy materials — ●KARSTEN W. JACOBSEN

Topical Talks of the Focused Session: Solid-liquid interfaces

- O 64.1 Thu 10:30–11:00 H31 **Cooperative Phenomena at the Solid/Liquid Interface** — ●KATHARINA KRISCHER
- O 64.3 Thu 11:15–11:45 H31 **Electrochemical energy conversion - interesting challenges for Surface Scientists** — ●HARRY E. HOSTER
- O 64.5 Thu 12:15–12:45 H31 **Interaction of Pt-nanoparticles with graphitic carbon structures - a computational study** — ●ALEXANDER A. AUER, WOLFGANG B. SCHNEIDER, UDO BENEDIKT
- O 76.1 Thu 16:00–16:30 H31 **The origin of the high oxygen reduction activity on PtX (X= Sc, Y, La, Sm, Gd and ..) alloys and their activation mechanism.** — ●IB CHORK-ENDORFF
- O 76.4 Thu 17:15–17:45 H31 **Coupling electrochemistry to an ICP-MS - online-investigation of electrode material dissolution** — ●KARL MAYRHOFER, SERHIY CHEREVKO, ANGEL TOPALOV, ANNA SCHUPPERT, JOSEF MEIER, ALEKSANDAR ZERADJANIN, IOANNIS KATSOUNAROS

Gaede Prize Talk

- O 47.1 Wed 13:15–13:55 H15 **Complex magnetic order on the atomic scale** — ●KIRSTEN VON BERGMANN

Invited talks of the joint symposium SYQP: Quantum Plasmonics (jointly with HL, TT)

See SYQP for the full program of the symposium.

- SYQP 1.1 Wed 15:00–15:30 H1 **Quantum plasmonics and applications in light harvesting** — ●PETER NORDLANDER
- SYQP 1.2 Wed 15:30–16:00 H1 **Deterministic quantum plasmonics with single nanodiamonds** — ●SERGE HUANT, ORIANE MOLLET, AURELIEN CUCHE, AURELIEN DREZET
- SYQP 1.3 Wed 16:00–16:30 H1 **Optically-active hybrid nanostructures: Exciton-plasmon interaction, Fano effect, and plasmonic chirality** — ●ALEXANDER GOVOROV
- SYQP 1.4 Wed 17:00–17:30 H1 **Quantum nano-optics: Interaction of metallic nano-particles with quantum emitters** — ●SALVATORE SAVASTA
- SYQP 1.5 Wed 17:30–18:00 H1 **Non-dipolar & magnetic interactions with optical antennas** — ALBERTO CURTO, MARTIN KUTTGE, MARTA CASTRO-LÓPEZ, ION HANCU, TIM TAMINIAU, ●NIEK VAN HULST

Invited talks of the joint symposium SYPM: Photons for Magnetism (jointly with MA, HL, MI)

See SYPM for the full program of the symposium.

- SYPM 1.1 Thu 15:00–15:30 H1 **Ultrafast emergence of nanoscale ferromagnetism far from equilibrium** — ●HERMANN DÜRR
- SYPM 1.2 Thu 15:30–16:00 H1 **Free-Electron Laser for Ultrafast Measurements in Material Science** — ●SVEN REICHE
- SYPM 1.3 Thu 16:00–16:30 H1 **Nanomagnetism seen by Femtosecond X-rays** — ●STEFAN EISEBITT
- SYPM 1.4 Thu 16:30–17:00 H1 **Ultrashort Radiation Pulses at Storage Rings** — ●HOLGER HUCK
- SYPM 1.5 Thu 17:00–17:30 H1 **Every atom counts - Magnetic properties of supported metal atoms and small alloy clusters** — TORBEN BEECK, IVAN BAEV, STEFFEN PALUTKE, KAI CHEN, SÖREN MEYER, KARI JÄNKÄLÄ, MICHAEL MARTINS, ●WILFRIED WURTH

Invited talks of the joint symposium SYES: Frontiers of electronic structure theory: Discovery of Novel Functional Materials (jointly with DS, HL, MA, MM, TT)

See SYES for the full program of the symposium.

- 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

O 1.1–1.1	Mon	9:30–10:15	H36	Invited Talk (Xiaoyang Zhu)
O 2.1–2.4	Mon	9:30–10:45	H10	Topological Insulators 1 (jointly with DS, HL, MA, TT)
O 3.1–3.7	Mon	9:30–11:15	H17	Graphene: Magnetic Fields (jointly with DS, HL, MA, and TT)
O 4.1–4.13	Mon	9:30–13:00	H20	Transport: Quantum Dots, Wires, Point Contacts 1 (jointly with HL and TT)
O 5.1–5.10	Mon	10:30–13:15	H36	Focussed Session: Frontiers of Electronic Structure Theory I (jointly with HL and TT)
O 6.1–6.10	Mon	10:30–13:00	H38	Organic/bio Molecules on Metal Surfaces I
O 7.1–7.10	Mon	10:30–13:00	H31	Plasmonics and Nanooptics I
O 8.1–8.11	Mon	10:30–13:15	H33	Surface Chemical Reactions and Heterogeneous Catalysis I
O 9.1–9.10	Mon	10:30–13:00	H42	Nanotribology
O 10.1–10.10	Mon	10:30–13:00	H45	Nanostructures at Surfaces I
O 11.1–11.9	Mon	11:30–13:45	H17	Graphene: Spin-orbit interaction (jointly with DS, HL, MA, and TT)
O 12.1–12.1	Mon	15:00–15:45	H36	Invited Talk (Swetlana Schauermaann)
O 13.1–13.11	Mon	15:00–19:20	H2	Focus Session: Crystalline n-type semiconducting oxides - SnO₂, Ga₂O₃, and In₂O₃ for novel devices (jointly with HL)
O 14.1–14.10	Mon	15:00–18:00	H10	Topological Insulators 2 (jointly with DS, HL, MA, TT)
O 15.1–15.5	Mon	15:00–17:45	H20	Focussed Session: Correlations in Topological Bands (jointly with DS, HL, MA, and TT)
O 16.1–16.5	Mon	15:00–17:30	H23	Magnetic Excitations: from surfaces down to adatoms (jointly with MA)
O 17.1–17.13	Mon	16:00–19:15	H36	Focussed Session: Frontiers of Electronic Structure Theory II (jointly with HL and TT)
O 18.1–18.12	Mon	16:00–19:00	H38	Organic/bio Molecules on Metal Surfaces II
O 19.1–19.12	Mon	16:00–19:00	H31	Plasmonics and Nanooptics II
O 20.1–20.12	Mon	16:00–19:00	H33	Surface Chemical Reactions and Heterogeneous Catalysis II
O 21.1–21.11	Mon	16:00–18:45	H42	Electronic Structure and Spin-Orbit Interaction I
O 22.1–22.11	Mon	16:00–18:45	H45	Nanostructures at Surfaces II
O 23.1–23.12	Mon	16:00–19:00	H17	Graphene: Electronic Properties and Transport (jointly with HL, MA and TT)
O 24.1–24.6	Mon	17:15–18:45	H32	Organic Electronics and Photovoltaics I (jointly with CPP, DS, HL)
O 25.1–25.1	Tue	9:30–10:15	H36	Invited Talk (Sohrab Ismail-Beigi)
O 26.1–26.12	Tue	9:30–12:45	H17	Transport: Graphene - Electronic Properties and Transport 2 (jointly with DS, HL, MA, and TT)
O 27.1–27.12	Tue	9:30–12:45	H32	Organic Electronics and Photovoltaics II (jointly with CPP, DS, HL)
O 28.1–28.10	Tue	10:30–13:15	H36	Focussed Session: Frontiers of Electronic Structure Theory III (jointly with HL and TT)
O 29.1–29.11	Tue	10:30–13:15	H38	Organic/bio Molecules on Metal Surfaces III
O 30.1–30.10	Tue	10:30–13:00	H31	Plasmonics and Nanooptics III
O 31.1–31.11	Tue	10:30–13:15	H33	Surface and Interface Magnetism I (jointly with MA)
O 32.1–32.8	Tue	10:30–12:30	H42	Metal Substrates I
O 33.1–33.9	Tue	10:30–12:45	H45	Nanostructures at Surfaces III
O 34.1–34.1	Tue	15:00–15:45	H36	Invited Talk (Martin Weinelt)
O 35.1–35.91	Tue	18:15–21:45	Poster B1	Poster Session I (Metal, semiconductor and oxide substrates: structure and adsorbates; Graphene)

O 36.1–36.89	Tue	18:15–21:45	Poster B2	Poster Session II (Organic films and electronics, photoorganics; Nanostructures; Plasmonics and nanooptics, Surface chemical reactions and heterogeneous catalysis, Surface dynamics)
O 37.1–37.1	Wed	9:30–10:15	H36	Invited Talk (Paul M. Koenraad)
O 38.1–38.14	Wed	9:15–13:00	H16	Topological Insulators (jointly with HL, MA, TT)
O 39.1–39.13	Wed	9:30–13:00	H17	Graphene: Characterization and Devices (jointly with DS, HL, MA, and TT)
O 40.1–40.10	Wed	9:30–12:15	H23	Spin Effects in Molecules at Surfaces (jointly with DS, MA)
O 41.1–41.11	Wed	10:30–13:30	H36	Focussed Session: Frontiers of Electronic Structure Theory IV (jointly with HL and TT)
O 42.1–42.11	Wed	10:30–13:15	H38	Organic/bio Molecules on Metal Surfaces IV
O 43.1–43.11	Wed	10:30–13:15	H31	Plasmonics and Nanooptics IV
O 44.1–44.11	Wed	10:30–13:15	H33	Scanning Probe Methods I
O 45.1–45.9	Wed	10:30–12:45	H42	Metal Substrates II
O 46.1–46.8	Wed	10:30–12:30	H45	Nanostructures and Clusters
O 47.1–47.1	Wed	13:15–13:55	H15	Gaede Prize Talk – Kirsten von Bergmann
O 48.1–48.1	Wed	15:00–15:45	H36	Invited Talk (Florian Klappenberger)
O 49.1–49.5	Wed	15:00–18:05	H1	Symposium Quantum Plasmonics (SYQP, jointly with HL, TT)
O 50.1–50.6	Wed	15:00–18:00	H20	Focussed Session: Majorana Fermions in Condensed Matter (jointly with DS, HL, MA, and TT)
O 51.1–51.13	Wed	16:00–19:30	H36	Focussed Session: Frontiers of Electronic Structure Theory V (jointly with HL and TT)
O 52.1–52.12	Wed	16:00–19:00	H38	Organic/bio Molecules on Metal Surfaces V
O 53.1–53.13	Wed	16:00–19:15	H31	Scanning Probe Methods II
O 54.1–54.12	Wed	16:00–19:00	H33	Organic Electronics and Photovoltaics (jointly with CPP, DS, HL)
O 55.1–55.13	Wed	16:00–19:15	H42	Electronic Structure and Spin-Orbit Interaction II
O 56.1–56.12	Wed	16:00–19:00	H45	Oxide Surfaces I
O 57.1–57.13	Wed	16:00–19:15	H17	Graphene: SiC Substrates and Intercalation (jointly with HL, MA and TT)
O 58.1–58.87	Wed	18:15–21:45	Poster B1	Poster Session III (Solid-liquid interfaces; Scanning probe and other methods; Electronic structure theory; Spin-orbit interaction)
O 59.1–59.1	Thu	9:30–10:15	H36	Invited Talk (Jörg Behler)
O 60.1–60.9	Thu	9:30–13:30	H32	Focussed Session: Organic Materials for Spintronics: From Spinterface to Devices (jointly with DS, HL, and MA)
O 61.1–61.12	Thu	9:30–13:00	H34	Organic Electronics and Photovoltaics I (jointly with CPP, DS, and HL)
O 62.1–62.10	Thu	10:30–13:15	H36	Focussed Session: Frontiers of Electronic Structure Theory VI (jointly with HL and TT)
O 63.1–63.10	Thu	10:30–13:00	H38	Plasmonics and Nanooptics V
O 64.1–64.6	Thu	10:30–13:00	H31	Focussed Session: Solid-liquid Interfaces I
O 65.1–65.10	Thu	10:30–13:00	H33	Surface and Interface Magnetism II (jointly with MA)
O 66.1–66.11	Thu	10:30–13:15	H42	Oxide Surfaces II
O 67.1–67.5	Thu	10:30–13:00	H45	Competition for the Gerhard Ertl Young Investigator Award
O 68.1–68.11	Thu	10:30–13:15	H17	Graphene: Preparation and Characterization I (jointly with HL, MA and TT)
O 69.1–69.1	Thu	15:00–15:45	H36	Invited Talk (Marc Koper)
O 70.1–70.5	Thu	15:00–17:30	H1	Symposium Photons in Magnetism (SYPM, jointly with MA, HL, MI)
O 71.1–71.13	Thu	15:00–18:45	H3	Surface Magnetism (jointly with MA)
O 72.1–72.9	Thu	15:00–17:30	H17	Graphene: Theory (jointly with DS, HL, MA, and TT)
O 73.1–73.13	Thu	15:00–18:45	H34	Organic Electronics and Photovoltaics II (jointly with CPP, DS, and HL)
O 74.1–74.12	Thu	16:00–19:00	H36	Focussed Session: Frontiers of Electronic Structure Theory VII (jointly with HL and TT)
O 75.1–75.13	Thu	16:00–19:15	H38	Organic/bio Molecules on Metal Surfaces VI
O 76.1–76.9	Thu	16:00–19:00	H31	Focussed Session: Solid-liquid Interfaces II
O 77.1–77.13	Thu	16:00–19:15	H33	Electronic Structure and Spin-Orbit Interaction III

O 78.1–78.13	Thu	16:00–19:15	H42	Surface Dynamics I
O 79.1–79.10	Thu	16:00–18:30	H45	Oxide Surfaces III
O 80	Thu	19:30–20:00	H36	Annual General Meeting of the Surface Science Division
O 81	Thu	20:00–21:00	H36	Post-Deadline Session
O 82.1–82.1	Fri	9:30–10:15	H36	Invited Talk (Richard Berndt)
O 83.1–83.5	Fri	9:30–12:00	H1	Symposium Frontiers of Electronic Structure Theory: Discovery of Novel Functional Materials (SYES, jointly with DS, HL, MA, MM and TT)
O 84.1–84.17	Fri	9:15–13:45	H2	Photovoltaics (jointly with CPP, DS and HL)
O 85.1–85.13	Fri	9:30–13:00	H18	Transport: Topological Insulators (jointly with DS, HL, MA, and TT)
O 86.1–86.10	Fri	10:30–13:00	H36	Plasmonics and Nanooptics VI
O 87.1–87.10	Fri	10:30–13:00	H31	Focussed Session: Solid-liquid Interfaces III
O 88.1–88.9	Fri	10:30–12:45	H38	Molecular Films
O 89.1–89.11	Fri	10:30–13:15	H33	Surface Dynamics II
O 90.1–90.11	Fri	10:30–13:15	H45	Semiconductor Substrates
O 91.1–91.10	Fri	10:30–13:00	H17	Graphene: Preparation and Characterization II (jointly with HL, MA and TT)
O 92.1–92.1	Fri	13:15–14:00	H36	Invited Talk (Helmut Zacharias)

Annual General Meeting of the Surface Science Division

Thursday 19:30–20:00 H36

- Report of the chairman
- Presentation of the Gerhard Ertl Young Investigator Award
- Miscellaneous

Post Deadline Session

Thursday 20:00–21:00 H36

Post Deadline Session followed by the Surface Science get-together.