

MM 12: Frontiers of Electronic Structure Theory: Focus on Topology and Transport

Monday 15:45–17:45

H51

Talk MM 12.1 Mon 15:45 H51
Mechanism of Li intercalation/deintercalation into/from the surface of LiCoO₂ — ●ASHKAN MORADABADI and PAYAM KAGHAZCHI — Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany

Talk MM 12.2 Mon 16:00 H51
Potential-dependent mechanism of Li diffusion in Li₂S — ●ASHKAN MORADABADI^{1,2} and PAYAM KAGHAZCHI¹ — ¹Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany — ²Institut für Materialwissenschaft, Fachgebiet Materialmodellierung, Technische Universität Darmstadt, Jovanka-Bontschits-Str. 2, 64287 Darmstadt, Germany

Talk MM 12.3 Mon 16:15 H51
Extremely high magnetoresistance in topological insulator candidate LaBi — ●NITESH KUMAR, CHANDRA SHEKHAR, and CLAUDIA FELSER — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany.

Talk MM 12.4 Mon 16:30 H51
VOTCA-STP - Multi Scale Modeling of Spin Transport in Organic Semiconductors — ●ERIK R. MCNELLIS, SHAYAN HEMMATIYAN, AMAURY MELO SOUZA, SEBASTIAN MÜLLER, and JAIRO SINOVA — Johannes Gutenberg University, Mainz, Germany

15 min. coffee break

Talk MM 12.5 Mon 17:00 H51
High-pressure and nonlinear elastic response of solids: Example of carbon allotropes — ●PASQUALE PAVONE, ROSTAM GOLESORKHTABAR, STEFAN KONTUR, and CLAUDIA DRAXL — Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, 12489 Berlin, Germany

Talk MM 12.6 Mon 17:15 H51
Calculations of temperature dependent resistivity for transition metals from the first principles — ●DAVID WAGENKNECHT^{1,2}, ILJA TUREK^{1,2}, and KAREL CARVA¹ — ¹Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University in Prague; Ke Karlovu 3, 12116 Prague 2, Czech Republic — ²Institute of Physics of Materials, Academy of Sciences of the Czech Republic; Žitkova 22, 61662 Brno, Czech Republic

Talk MM 12.7 Mon 17:30 H51
Ab Initio Molecular Dynamics Study of Conjugated Polymer Systems: The Elusive Localization of the Polaron — ●HÅKAN W. HUGOSSON¹, AMINA MIRSAKIYEVA¹, and ANNA DELIN^{1,2} — ¹Department of Materials och Nano Physics, KTH Royal Institute of Technology, Stockholm, Sweden. — ²Ångström Laboratory, Uppsala University, Uppsala, Sweden.

O 41: Frontiers of Electronic Structure Theory: Focus on Topology and Transport I

Tuesday 14:00–16:00

H24

Topical Talk O 41.1 Tue 14:00 H24
Topological semimetals and chiral transport in inversion asymmetric systems — ●SHUICHI MURAKAMI — Department of Physics and TIES, Tokyo Institute of Technology, Tokyo, Japan

Talk O 41.2 Tue 14:30 H24
Topological orbital magnetic moments — ●MANUEL DOS SANTOS DIAS, JUBA BOUAZIZ, MOHAMMED BOUHASSOUNE, STEFAN BLÜGEL, and SAMIR LOUNIS — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Talk O 41.3 Tue 14:45 H24
The orbital Rashba effect — ●DONGWOOK GO^{1,2}, PATRICK BUHL¹, GUSTAV BIHLMAYER¹, YURIY MOKROUSOV¹, HYUN-WOO LEE², and STEFAN BLÜGEL¹ — ¹Institute for Advanced Simulation and Peter Grünberg Institut, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — ²Department of Physics, Pohang University of Science and Technology, 37673 Pohang, Korea

Talk O 41.4 Tue 15:00 H24
Spin and orbital magnetism of Rashba electrons induced by magnetic nanostructures — ●JUBA BOUAZIZ, MANUEL DOS SANTOS DIAS, PHIVOS MAVROPOULOS, STEFAN BLÜGEL, and SAMIR LOUNIS

— Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Talk O 41.5 Tue 15:15 H24
First-principles investigation of the impact of single atomic defects on magnetic skyrmions — ●IMARA L. FERNANDES, BENEDIKT SCHWEFLINGHAUS, JUBA BOUAZIZ, STEFAN BLÜGEL, and SAMIR LOUNIS — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany

Talk O 41.6 Tue 15:30 H24
Topological magnons: Any chance to find them? — ●ALEXANDER MOOK¹, JÜRGEN HENK², and INGRID MERTIG^{1,2} — ¹Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle — ²Institut für Physik, Martin-Luther-Universität, D-06120 Halle

Talk O 41.7 Tue 15:45 H24
Acoustic magnons in the long-wavelength limit: resolving the Goldstone violation in many-body perturbation theory — ●MATHIAS C.T.D. MÜLLER, CHRISTOPH FRIEDRICH, and STEFAN BLÜGEL — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

O 55: Frontiers of Electronic Structure Theory: Focus on Topology and Transport II

Wednesday 10:30–13:00

H24

Talk O 55.1 Wed 10:30 H24
Coupled-Cluster approach for both molecules and solids in the numeric atom-center orbital framework — ●TONGHAO SHEN, ARVID CONRAD IHRIG, IGOR YING ZHANG, and MATTHIAS SCHEFFLER — *Fritz-Haber-Institut der MPG, Berlin.*

Talk O 55.2 Wed 10:45 H24
Surface adsorption energetics at the "gold standard": Small molecule binding to TiO₂(110) — ●DANIEL BERGER^{1,2}, A. KUBAS³, D. MANGANAS³, H. OBERHOFER¹, F. NEESE³, and K. REUTER¹ — ¹TU München — ²University of California, Los Angeles — ³MPI für chemische Energiekonversion, Mülheim an der Ruhr

Talk O 55.3 Wed 11:00 H24
Water adsorption on surfaces form many-body perturbation theory — ●THEODOROS TSATSOULIS and ANDREAS GRÜNEIS — Max-Planck-Institute for Solid State Research, Stuttgart

Talk O 55.4 Wed 11:15 H24
Photo-isomerization in azobenzene-functionalized self-assembled monolayers: The impact of many-body effects — ●CATERINA COCCHI and CLAUDIA DRAXL — Institut für Physik und IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

Talk O 55.5 Wed 11:30 H24

Laplace-transformed MP2 with localized Resolution of Identity -efficient in-memory MP2 for large systems — ●ARVID CONRAD IHRIG¹, PATRICK RINKE², IGOR YING ZHANG¹, and MATTHIAS SCHEFFLER¹ — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — ²Aalto University, Helsinki, Finland

Talk O 55.6 Wed 11:45 H24
GW singles contributions for the random phase approximation correlation energies — ●JIRI KLIMES¹, MERZUK KALTAK², EMANUELE MAGGIO³, and GEORG KRESSE³ — ¹J. Heyrovský Institute of Physical Chemistry, Prague, Czech Republic — ²Department of Physics and Astronomy, Stony Brook University, Stony Brook, NY — ³University of Vienna, Faculty of Physics, Vienna, Austria

Talk O 55.7 Wed 12:00 H24
Long-range corrected DFT meets GW: Vibrationally resolved photoelectron spectra from first principles — ●THOMAS KÖRZDÖRFER — Institut für Chemie, Universität Potsdam, D-14476 Potsdam

Talk O 55.8 Wed 12:15 H24
LDA-1/2 as a starting point for G_0W_0 calculations — ●RONALDO RODRIGUES PELA^{1,2}, UTE WERNER¹, DMITRII NABOK¹, and CLAUDIA DRAXL¹ — ¹Humboldt-Universität zu Berlin, Institut für Physik and IRIS Adlershof, Berlin, Germany — ²Instituto Tecnológico de Aeronáutica, São José dos Campos, Brazil

Talk O 55.9 Wed 12:30 H24
DFT+U within a numeric atom-centered orbital basis — ●MATTHIAS KICK, HARALD OBERHOFER, and KARSTEN REUTER — Technische Universität München

Talk O 55.10 Wed 12:45 H24
High-throughput Screening and Statistical Learning for Design of Transparent Conducting Oxides — ●CHRISTOPHER SUTTON, LUCA M. GHIRINGHELLI, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der Max-Planck-Gesellschaft

O 62: Frontiers of Electronic Structure Theory: Focus on Topology and Transport III

Wednesday 15:00–18:30

H24

Topical Talk O 62.1 Wed 15:00 H24
Topological semimetal phases in strained HgTe-based alloys — TOMÁŠ RAUCH¹, STEVEN ACHILLES¹, ●JÜRGEN HENK¹, and INGRID MERTIG^{1,2} — ¹Martin Luther University Halle-Wittenberg, Halle, Germany — ²Max Planck Institute of Microstructure Physics, Halle, Germany

Topical Talk O 62.2 Wed 15:30 H24
Topological surface Fermi arcs and the chiral anomaly in Weyl semimetal materials — ●BINGHAI YAN — Max Planck Institute for Chemical Physics of Solids, Dresden

Talk O 62.4 Wed 16:15 H24
Topological surface Fermi arcs and spin-textures of the Weyl semimetals TaAs, TaP, NbAs, and NbP — ●YAN SUN¹, SHU-CHUN WU¹, CLAUDIA FELSER¹, and BINGHAI YAN^{1,2} — ¹Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany. — ²Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany

Talk O 62.5 Wed 16:30 H24
New electron states at the Bi/InAs(111) interface — ●L NICOLAÏ^{1,2,3}, K HRICOVINI^{2,3}, J-M MARIOT⁴, M C RICHTER^{2,3}, O HECKMANN^{2,3}, U DJUKIC², T BALASUBRAMANIAN⁵, M LEANDERSSON⁵, J SADOWSKI⁵, J DENLINGER⁶, I VOBORNIK⁷, J BRAUN⁷, H EBERT⁷, and J MINÁR^{7,8} — ¹LMU, Munich — ²LPMS, UCP, Cergy, France — ³DSM-IRAMIS, Spec, Cea-Saclay, France — ⁴LCP-MR, UPMC Univ. Paris 06/CNRS, France — ⁵MAX-lab, Lund Univ., Sweden — ⁶ALS, Berkeley, USA — ⁷EST, Trieste, Italy — ⁸Univ. of West Bohemia, Plzeň, Czech Republic

Talk O 62.6 Wed 16:45 H24
Two-dimensional topological phases and electronic spectra of topological insulator thin films from GW calculations — ●TOBIAS FÖRSTER, PETER KRÜGER, and MICHAEL ROHLFING — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

Talk O 62.7 Wed 17:00 H24

Steady-State Density Functional Theory for Finite Bias Conductances — ●STEFAN KURTH^{1,2} and GIANLUCA STEFANUCCI^{3,4} — ¹Dept. of Materials Physics, Univ. of the Basque Country UPV/EHU, San Sebastian, Spain — ²IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — ³Dept. of Physics, Univ. of Rome "Tor Vergata", Rome, Italy — ⁴INFN, Frascati, Italy

Talk O 62.8 Wed 17:15 H24
Revealing the intra-molecular origin of inelastic electron tunneling signal by means of first-principles calculations — ●GIUSEPPE FOTI and HECTOR VAZQUEZ — Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnicka 10, Prague, Czech Republic

Talk O 62.9 Wed 17:30 H24
An efficient real-time time-dependent density functional theory method and its applications — ●ZHI WANG¹, SHU-SHEN LI², and LIN-WANG WANG³ — ¹Institut für Physikalische Chemie, Uni-Hamburg, Hamburg, Germany — ²Institute of Semiconductors, Chinese Academy of Sciences, Beijing, China — ³Lawrence Berkeley National Laboratory, Berkeley, United States

Talk O 62.10 Wed 17:45 H24
Nonadiabatic geometric phase of a pseudorotating triatomic molecule — ●RYAN REQUIST and EBERHARD K. U. GROSS — Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

Talk O 62.11 Wed 18:00 H24
Theoretical investigations of magnetically doped topological insulators — ●JAN MINAR^{1,2}, JURGEN BRAUN¹, and HUBERT EBERT¹ — ¹LMU München, Germany — ²University of West Bohemia, Plzen, Czech Rep.

Talk O 62.12 Wed 18:15 H24
Trions in a carbon nanotube from ab-initio many-body perturbation theory — ●THORSTEN DEILMANN, MATTHIAS DRÜPPEL, and MICHAEL ROHLFING — Institut für Festkörpertheorie, Universität Münster, Germany

O 66: Frontiers of Electronic Structure Theory: Focus on Topology and Transport

Wednesday 18:15–20:30

Poster A

Poster O 66.1 Wed 18:15 Poster A
Improving anharmonic vibrational calculations from first principles — ●JOSEPH C.A. PRENTICE, BARTOMEU MONSERRAT, and RICHARD J. NEEDS — TCM Group, Cavendish Laboratory, University of Cambridge, UK

Poster O 66.2 Wed 18:15 Poster A
Towards a practical implementation of second-order Møller-Plesset perturbation theory for solids — ●XIANGYUE LIU, ARVID CONRAD IHRIG, SERGEY LEVCHENKO, IGOR YING ZHANG, and MATTHIAS SCHEFFLER — *Fritz-Haber-Institut der MPG, Berlin, DE*

Poster O 66.3 Wed 18:15 Poster A
Application of the exact exchange functional to magnetic metals within the FLAPW method — ●MAX NUSSPICKEL¹, MARKUS BETZINGER¹, CHRISTOPH FRIEDRICH¹, ANDREAS GÖRLING², and STEFAN BLÜGEL¹ — ¹Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany — ²Lehrstuhl für Theoretische Chemie, Universität Erlangen-Nürnberg, Germany

Poster O 66.4 Wed 18:15 Poster A
Electric switchable giant Rashba-type spin splitting in bulk

PbS — ●BIN SHAO¹, WENHUI DUAN², and THOMAS FRAUENHEIM¹ — ¹BCCMS, University of Bremen, Bremen, Germany — ²Institute for Advanced Study, Tsinghua University, Beijing, China

Poster O 66.5 Wed 18:15 Poster A
GW+fRG: Towards an fRG enhancement of ab initio calculations — ●JANNIS EHRLICH^{1,2}, CARSTEN HONERKAMP¹, CHRISTOPH FRIEDRICH², and STEFAN BLÜGEL² — ¹Institut für theoretische Festkörperphysik, RWTH Aachen University, D-52056 Aachen, Germany — ²PGI-1 and IAS-1, FZJ & JARA, D-52425 Jülich, Germany

Poster O 66.6 Wed 18:15 Poster A
The quantum anomalous Hall effect in HgMnTe — ●JAN BÖTTCHER, CHRISTOPH KLEINER, and EWELINA M. HANKIEWICZ — Uni Würzburg, Institut für Theoretische Physik und Astrophysik, Germany

Poster O 66.7 Wed 18:15 Poster A
Nonconventional screening of the Coulomb interaction in low-dimensional semiconductors and insulators — ERSOY SASIOGLU, ●CHRISTOPH FRIEDRICH, and STEFAN BLÜGEL — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

O 80: Frontiers of Electronic Structure Theory: Focus on Topology and Transport IV

Thursday 10:30–13:15

H24

Topical Talk O 80.1 Thu 10:30 H24
Transport phenomena in broken-symmetry metals: Geometry, topology, and beyond — ●IVO SOUZA — Universidad del País Vasco, San Sebastián, Spain

Topical Talk O 80.2 Thu 11:00 H24
Dirac Fermions in Antiferromagnetic Semimetal — ●PEIZHE TANG, QUAN ZHOU, GANG XU, and SHOU-CHENG ZHANG — Department of Physics, McCullough Building, Stanford University, Stanford, California 94305-4045, USA

Talk O 80.3 Thu 11:30 H24
Spin Hall effect in non-collinear antiferromagnets Mn₃X (X=Sn, Ge, Ga) — ●YANG ZHANG^{1,3}, YAN SUN¹, CLAUDIA FELSER¹, and BINGHAI YAN^{1,2} — ¹Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — ²Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — ³Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany

Talk O 80.4 Thu 11:45 H24
Electronic reconstruction and anomalous Hall conductivity in 3d-oxide honeycomb lattices within the corundum structure — ●SANTU BAIDYA and ROSSITZA PENTCHEVA — Fakultät für Physik and Center of Nanointegration (CENIDE), Universität Duisburg-Essen, 47057 Duisburg

Talk O 80.5 Thu 12:00 H24
Anomalous hall effect in triangular antiferromagnetic ordered structure — ●HAO YANG¹, SUN YAN², FELSER CLAUDIA², PARKIN

STUART¹, and BINGHAI YAN² — ¹Max Planck Institute of Microstructure Physics, 06120 Halle(Saale), Germany — ²Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

Talk O 80.6 Thu 12:15 H24
Anomalous Hall conductivity and orbital magnetization as local quantities — ●ANTIMO MARRAZZO¹ and RAFFAELE RESTA² — ¹THEOS, EPF Lausanne, Switzerland — ²Dipartimento di Fisica, Univ. Trieste, Italy

Talk O 80.7 Thu 12:30 H24
Laser induced DC photocurrents in a Topological Insulator thin film — ●THOMAS SCHUMANN¹, NINA MEYER¹, GREGOR MUSSLER⁴, EVA SCHMORANZEROVÁ², DAGMAR BUTKOVICOVA², HELENA REICHLIOVÁ³, LUKAS BRAUN⁵, CHRISTIAN FRANZ⁶, MICHAEL CZERNER⁶, PERTR NĚMEC², DETLEV GRÜTZMACHER⁴, TOBIAS KAMPFRATH⁵, CHRISTIAN HEILIGER⁶, and MARKUS MÜNZENBERG¹ — ¹IIP, EMA University Greifswald, Germany — ²MFF, Charles University, Prague, Czech Republic — ³FZU, Prague, Czech Republic — ⁴PGI-9, Jülich, Germany — ⁵FHI Berlin, Germany — ⁶University of Gießen, Germany

Talk O 80.8 Thu 12:45 H24
Robustness of exchange protocols of Majorana fermions in quantum wire networks — ●CHRISTIAN TUTSCHKU¹, ROLF W. REINTHALER¹, CHAO LEI², ALLAN H. MACDONALD², and EWELINA M. HANKIEWICZ¹ — ¹Faculty of Physics and Astrophysics, University of Würzburg, Würzburg, Germany — ²Department of Physics, University of Texas at Austin, USA

O 88: Frontiers of Electronic Structure Theory: Focus on Topology and Transport V

Thursday 15:00–18:15

H24

Talk O 88.2 Thu 15:15 H24
All-Electron Many-Body Approach to X-Ray Absorption Spectroscopy — ●CHRISTIAN VORWERK, CATERINA COCCHI, and CLAUDIA DRAXL — Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

Talk O 88.3 Thu 15:30 H24
Cohesive properties from all-electron RPA total energies — ●MARKUS BETZINGER¹, CHRISTOPH FRIEDRICH¹, ANDREAS GÖRLING², and STEFAN BLÜGEL¹ — ¹Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany — ²Lehrstuhl für Theoretische Chemie, Universität Erlangen-Nürnberg, Germany

Talk O 88.4 Thu 15:45 H24
Explicitly correlated self consistent field theory — ●CHRISTIAN LASAR and THORSTEN KLÜNER — Universität Oldenburg

Talk O 88.5 Thu 16:00 H24
Representing energy landscapes by combining neural networks and the empirical valence bond method — ●SINJA KLEES¹, RAMONA UFER², VOLODYMYR SERGHEVSKYI², ECKHARD SPOHR², and JÖRG BEHLER¹ — ¹Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany — ²Lehrstuhl für Theoretische Chemie, Universität Duisburg-Essen, D-45141 Essen, Germany

Talk O 88.6 Thu 16:15 H24
CELL: a python package for cluster expansions with large parent cells — ●SANTIAGO RIGAMONTI¹, MARIA TROPPEZ¹, CHRISTOPHER SUTTON², LUCA M. GHIRINGHELLI², and CLAUDIA DRAXL¹ — ¹Humboldt-Universität zu Berlin — ²Fritz-Haber-Institut der Max-Planck-Gesellschaft

Talk O 88.7 Thu 16:30 H24
Structural and electronic properties of the thermoelectric clathrates Ba₈Al_xSi_{46-x} and Sr₈Al_xSi_{46-x} — ●MARIA TROPPEZ, SANTIAGO RIGAMONTI, and CLAUDIA DRAXL — Humboldt-Universität zu Berlin

Talk O 88.8 Thu 16:45 H24

Ab-initio calculation of Raman spectra of graphene-based materials — ●ALBIN HERTRICH, CATERINA COCCHI, PASQUALE PAVONE, and CLAUDIA DRAXL — Department of Physics, Humboldt-Universität zu Berlin, Germany

Talk O 88.9 Thu 17:00 H24
Exciton dispersion in layered and 2D systems — ●FRANCESCO SOTTILE^{1,2}, GIORGIA FUGALLO^{1,2}, PIERLUIGI CUDAZZO^{1,2}, and MATTEO GATTI^{1,2,3} — ¹Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-IRAMIS, Université Paris-Saclay, F-91128 Palaiseau, France — ²European Theoretical Spectroscopy Facility — ³Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin, Boîte Postale 48, F-91192 Gif-sur-Yvette, France

Talk O 88.10 Thu 17:15 H24
Electronic structure of selected superheavy elements (Z_i104) — ●HANA CENCARIKOVA¹ and DOMINIK LEGUT² — ¹Institute of Experimental Physics, SAS, Kosice, Slovakia — ²IT4Innovations Center, VSB-TU Ostrava, CZ 708 33 Ostrava, Czech Republic

Talk O 88.11 Thu 17:30 H24
Layer-resolved calculated vibrations at gold surfaces — ●ANDREI POSTNIKOV¹ and KAMIL MOLDOŠANOV² — ¹Université de Lorraine, LCP-A2MC, Metz, France — ²Kyrgyz-Russian Slavic University, Bishkek, Kyrgyzstan

Talk O 88.12 Thu 17:45 H24
Electronic structure, mechanical and thermodynamic properties of Actinium from first-principles — ●BARBORA KACEROVSKA¹ and DOMINIK LEGUT² — ¹Nanotechnology, VSB-TU Ostrava, CZ 708 33 Ostrava, Czech Republic — ²IT4Innovations Center, VSB-TU Ostrava, CZ 708 33 Ostrava, Czech Republic

Talk O 88.13 Thu 18:00 H24
Interaction of Tritium and Chlorine 36 with defects in Graphite: Insights from Theory — ●CHRISTOPH LECHNER¹, PHILIPPE BARANEK¹, and HOLGER VACH² — ¹EDF Lab Les Renardières, Avenue des Renardières, F-77818 Moret-sur-Loing Cedex, France — ²CNRS-LPICM, Ecole Polytechnique, F-91128 Palaiseau Cedex, France

O 99: Symposium on Frontiers of Electronic Structure Theory: Focus on Topology and Transport

Friday 09:30–12:15

H1

Invited Talk O 99.1 Fri 9:30 H1
Intrinsic Transport Coefficients and Momentum Space Berry Curvatures — ●ALLAN H MACDONALD — University of Texas at Austin, Austin TX, USA

Invited Talk O 99.2 Fri 10:00 H1
Berry phase linked spin-orbit torques in Ferromagnetic and Antiferromagnetic systems — ●JAIRO SINOVA — Johannes Gutenberg Universität Mainz, Staudingerweg 7, 55128 Mainz Germany

Invited Talk O 99.3 Fri 10:30 H1
Transport in Topological Insulators and Topological Superconductors: In Search of Majorana Fermions — ●EWELINA HAN-

KIEWICZ — Wuerzburg University

session break

Invited Talk O 99.4 Fri 11:15 H1
Engineering Topological Quantum States: From 1D to 2D. — ●JELENA KLINOVAJA — University of Basel, Switzerland

Invited Talk O 99.5 Fri 11:45 H1
Skyrmions – Topological magnetization solitons for future spintronics — ●STEFAN BLÜGEL — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany