Program

Monday, August 21

15.00 - 23.00	Registration at Åkerblads gästgiveri
15.30 - 17.00	Coffee and refreshments at Åkerblads gästgiveri
19.00 - 22.00	Get together barbecue buffet at Lake Siljan Welcome speech by Olle Eriksson (Uppsala University, Sweden)

Tuesday, August 22

Morning Plenary Session
Room: Oppsittu
Chair: Levente Vitos

8.30 - 8.40	Opening (Levente Vitos)
8.40 - 9.20	**Ann E. Mattsson**, Sandia National Laboratories, Albuquerque, USA *A density based Electron Localization Function*
9.20 - 10.00	**Ursula Röthlisberger**, Swiss Federal Institute of Technology in Lausanne, Switzerland *Nature knows best: computational strategies for the design of biomimetic systems*
10.00 - 10.30	Coffee & refreshments break

Morning Invited Session A (parallel)
Room: Oppsittu
Chair: Martin Kaupp

10.30 - 11.00	**Julien Toulouse**, Université Pierre-et-Marie-Curie, Paris, France *Combining density-functional theory and many-body methods*
11.00 - 11.30	**Weitao Yang**, Duke University, Durham, USA *Localized Orbital Scaling Correction for Systematic Elimination of Delocalization Error in Density Functional Approximations*
11.30 - 12.00	**Marcus, Elstner**, Karlsruhe Institute of Technology, Germany *The approximate DFT models 'DFTB': performance and challenges*
12.00 - 12.30	**Henryk, Witek**, National Chiao Tung University, Hsinchu, Taiwan *Automatized parameterization of DFTB*

Morning Invited Session B (parallel)
Room: Rådstuggu
Chair: Juan-Carlos Sancho-Garcia

10.30 - 11.00 **Per Hyldgaard**, Chalmers University of Technology, Sweden
Understanding exchange and correlation in regular and hybrid van der Waals density functionals

11.00 - 11.30 **Vincent Tognetti**, University of Rouen, France
The DFT-CDFT-QTAIM synergy to investigate chemical reactivity

11.30 - 12.00 **Frank De Proft**, Vrije Universiteit Brussel, Brussels, Belgium
Chemical Concepts from Density Functional Theory: Theoretical Developments and Applications in Bonding, Chemical Reactivity and Molecular Design

12.00 - 12.30 **Kersti Hermansson**, Uppsala University, Sweden
DFT-based multi-scale modelling of materials and nanoparticles

12.30 - 14.00 Lunch at Åkerblads gästgiveri

Afternoon Invited Session A (parallel)
Room: Oppsittu
Chair: Peter Mohn

14.00 - 14.30 **Ferdi Aryasetiawan**, Lund University, Sweden
Hubbard bands vs plasmons in correlated metals: A view from self-consistent GW+DMFT

14.30 - 15.00 **Liviu Chioncel**, Augsburg University, Germany
Towards multiple-scattering theory for disordered systems with Anderson localization

15.00 - 15.30 **Manuel Richter**, IFW Dresden, Germany
Quantitative Predictions by Electronic Structure Theory

Afternoon Invited Session B (parallel)
Room: Rådstuggu
Chair: Kersti Hermansson

14.00 - 14.30 **Hiromi Nakai**, Waseda University, Tokyo, Japan
Relativistic density functional theory with picture-change corrected electron density based on infinite-order Douglas-Kroll-Hess method

14.30 - 15.00 **Trond Saue**, Université Toulouse III-Paul Sabatier, France
Beyond the electric dipole approximation in simulations of X-ray absorption spectroscopy

15.00 - 15.30 **Andrew Teale**, University of Nottingham, UK
Density-Functional Theory for Molecules in Strong Magnetic Fields

15.30 - 16.00 Coffee & refreshments break

Afternoon Plenary Session
Room: Oppsittu
Chair: John Wills

16.00 - 16.40 **John Perdew**, Temple University, Philadelphia, USA
The SCAN Density Functional: Nonempirical, Predictive, and Efficient

Contributed Session A (parallel)
Room: Oppsittu
Chair: John Wills

16.45 - 17.00 **Andreas Östlin**, Augsburg University, Germany
Green's function-based method for correlated electronic structure calculations

17.00 - 17.15 **Li Huang**, China Academy of Engineering Physics, Jiangyou, China
Combined semilocal exchange potential with dynamical mean-field theory

17.15 - 17.30 **David O'Regan**, Trinity College Dublin, Ireland
Optimizing constraints and corrections in approximate DFT

17.30 - 17.45 **Chandre Dharma-wardana**, National Research Council of Canada, Ottawa, Canada
Finite-T electron-electron, electron-ion and ion-ion xc-functionals, discontinuities in the mean ionization, and phase transitions in low-Z warm-dense matter

Contributed Session B (parallel)
Room: Rådstuggu
Chair: Kalevi Kokko

16.45 - 17.00 **Eduardo Fabiano**, Italian National Research Council, Lecce, Italy
The interaction-strength interpolation method for main-group chemistry: benchmarking, limitations, and perspectives

17.00 - 17.15 **Yang Jiao**, Chalmers University of Technology, Sweden
Towards truly nonlocal exchange and correlation functionals: Nonempirical constructions

17.15 - 17.30 **Thilo Aschebrock**, University of Bayreuth, Germany
Semi-local exchange functionals showing ultranonlocal response: the hope to replace exact exchange

17.30 - 17.45 **Peter Blaha**, TU Vienna, Austria
A simple way to apply nonlocal van der Waals functionals within all-electron methods

19.00 - 20.30 Dinner at Åkerblads gästgiveri

Poster Session
Room: Storstuga
Chair: Henry Chermette, Claude A. Daul

20.30 - 22.00 **Posters A** (Poster presenters on p. 11)

Wednesday, August 23

Memorial Session
Room: Oppsittu
Chair: Ágnes Nagy

8.00 - 8.40	**Claude A. Daul, Karlheinz Schwarz, Ann E. Mattsson, and Mel Levy**, *Presentation in memory of Annick Leray-Goursot and Walter Kohn*

Plenary Session
Room: Oppsittu
Chair: Ágnes Nagy

8.40 - 9.20	**Mel Levy**, Duke University, Durham, USA *Exact Constraints for Creating Density Functionals, and Thoughts of Robert G. Parr*
9.20 - 10.00	**Trygve Helgaker**, University of Oslo, Norway *The Four-Way Correspondence of Density-Functional Theory*
10.00 - 10.30	Coffee & refreshments break

Invited Session A (parallel)
Room: Oppsittu
Chair: Weitao Yang

10.30 - 11.00	**Kieron Burke**, University of California, Irvine, USA *Direct extraction of excitation energies from ensemble density-functional theory*
11.00 - 11.30	**Aron Cohen**, University of Cambridge, UK *The Exact Density Functional*
11.30 - 12.00	**Neepa Maitra**, Hunter College of the City University of New York, USA *New Approaches to Memory-Dependent Functionals in Time-Dependent Density Functional Theory*
12.00 - 12.30	**Michael Peach**, Lancaster University, UK *Triplet Emission Processes in Platinum Complexes*

Invited Session B (parallel)
Room: Rådstuggu
Chair: Hiromi Nakai

10.30 - 11.00	**Éric Brémond**, CompuNet, Istituto Italiano di Tecnologia, Italy *Single and Double Hybridization Schemes in Density-Functional Theory*
11.00 - 11.30	**Juan Carlos Sancho-Garcia**, University of Alicante, Spain *Benchmark and Applications Studies of Double-Hybrid Density Functionals Based on the Adiabatic Connection Model*
11.30 - 12.00	**Martin Kaupp**, Technical University of Berlin, Germany *Recent Progress on Local Hybrid Functionals*
12.00 - 12.30	**Andreas M. Köster**, CINVESTAV, Mexico City, Mexico *Hybrid Functionals in Auxiliary Density Function Theory*

12.30 - 14.00 Lunch at Åkerblads gästgiveri

Contributed Session A (parallel)
Room: Oppsittu
Chair: Paola Gori-Giorgi

14.00 - 14.15 **Thomas Niehaus**, Université Lyon, France
The budget way to quasiparticle and exciton binding energies

14.15 - 14.30 **Klaas Giesbertz**, Vrije Universiteit Amsterdam, The Netherlands
Invertibility of the retarded response functions for initial mixed states: application to one-body reduced density matrix functional theory

14.30 - 14.45 **Ireneusz Grabowski**, Nicolaus Copernicus University, Poland
Optimized Effective Potential Method based on the Scaled-Opposite-Spin Second-Order Correlation

14.45 - 15.00 **Michael G. Medvedev**, A. N. Nesmeyanov Institute of Organoelement Compounds of Russian Academy of Sciences, Moscow, Russia
Accuracy of DFT self-consistent electron densities

15.00 - 15.15 **Eduard Matito**, Donostia International Physics Center, Bilbao, Spain
DFT functional assessment from quasi-exact energies and densities at different correlation regimes

15.15 - 15.30 **Patrizia Calaminici**, CINVESTAV, Mexico
On the Structure Determination of U_2C_79: U_2CC_{78} or $U_2C_3C_{76}$? Insight from a DFT Study

Contributed Session B (parallel)
Room: Rådstuggu
Chair: Miguel Marques

14.00 - 14.15 **Luis Cort Barrada**, University of Jyväskylä, Finland
Time-dependent density-functional theory for strongly interacting electrons

14.15 - 14.30 **Lionel Lacombe**, Hunter College of the City University of New York, USA
Modeling the exact time-dependent exchange-correlation potential

14.30 - 14.45 **Peter Elliott**, Max-Planck Institute of Microstructure Physics, Germany
Ultrafast Charge and Spin Dynamics with TDDFT

14.45 - 15.00 **Mauro Stener**, University of Trieste, Italy
A New Efficient Time Dependent Density Functional Algorithm for Large Systems: Theory, Implementation and Plasmonics Applications

15.00 - 15.15 **Eloy Ramos-Cordoba**, University of California, Berkeley, USA
Excited states for orbital-optimized second-order perturbation theory

15.15 - 15.30 **Kristian Berland**, University of Oslo, Norway
An assessment of hybrid functionals for transport and excited-state properties of bulk semiconductors

15.30 - 16.00 Coffee & refreshments break

Excursion

16.00 - 19.00	Guided church boat excursion on lake Siljan *or* guided tour to Digerberget (Diger summit)
19.30 - 21.00	Conference dinner at Åkerblads gästgiveri Presentation about Dalarna by Börje Johansson (KTH - Royal Institute of Technology, Stockholm, Sweden)

Poster Session
Room: Storstuga
Chair: Jose Garcia de la Vega, Paul Geerlings

21.00 - 22.30	**Posters B** (Poster presenters on p. 13)

Thursday, August 24

Plenary Session
Room: Oppsittu
Chair: Kieron Burke

8.40 - 9.20	**Robert van Leeuwen**, University of Jyväskylä, Finland *The density-potential mapping in time-dependent density-functional theory*
9.20 - 10.00	**Matthias Ernzerhof**, University of Montreal, Canada *Constructing exchange-correlation functionals using the strong-interaction limit and the correlation factor ansatz*
10.00 - 10.30	Coffee & refreshments break

Morning Invited Session A (parallel)
Room: Oppsittu
Chair: Leonid Sandratskii

10.30 - 11.00	**Kalevi Kokko**, University of Turku, Finland *Quasi non-uniform approximation, flexible exchange-correlation functional for alloys and compounds*
11.00 - 11.30	**Zhimei Sun**, Beihang University, Beijing, China *Electronic and topological properties of MXenes: a first-principles study*
11.30 - 12.00	**Balazs Ujfalussy**, Wigner Research Center for Physics, Budapest, Hungary *Superconducting order parameter in layered systems*
12.00 - 12.30	**Qing-Miao Hu**, Institute of Metal Research, Shenyang, China *Applications of Density Functional Theory on Design of Advanced Titanium Alloys*

Morning Invited Session B (parallel)
Room: Rådstuggu
Chair: Trond Saue

10.30 - 11.00	**Jing Kong**, Middle Tennessee State University, Murfreesboro, USA *Density Functional for Computing the Strong Nondynamic Correlation*
11.00 - 11.30	**John M. Wills**, Los Alamos National Laboratory, USA *Automatic generation of pseudopotentials by an all-electron methods*
11.30 - 12.00	**Rickard Armiento**, Linköping University, Sweden *Semi-Local Functionals with Non-vanishing Asymptotic Potentials: Beyond the AK13*
12.00 - 12.30	**Jijun Zhao**, Dalian University of Technology, China *Which is the best exchange-correlation functional for describing atomic and molecular clusters?*
12.30 - 14.00	Lunch at Åkerblads gästgiveri

Afternoon Invited Session A (parallel)
Room: Oppsittu
Chair: Balazs Ujfalussy

14.00 - 14.30	**Alexander Landa**, Lawrence Livermore National Laboratory, USA *Alloying-Driven Phase Stability in Group-VB Transition Metals Under Compression*
14.30 - 15.00	**Per Söderlind**, Lawrence Livermore National Laboratory, USA *Phase stability, elasticity, and phonons for plutonium from electronic-structure theory*
15.00 - 15.30	**Peter Mohn**, Vienna University of Technology, Austria *Ab initio calculation of spin lattice relaxation of NV^- centers in diamond*

Afternoon Invited/Contributed Session B (parallel)
Room: Rådstuggu
Chair: Henryk Witek

14.00 - 14.30	**Claudio Amovilli**, University of Pisa, Italy *Properties of electron density in weak binding conditions*
14.30 - 15.00	**Leonid Sandratskii**, Max Planck Institute of Microstructure Physics, Halle, Germany *The insight into the Dzyaloshinskii-Moriya interaction through first-principles study of chiral magnetic structures*
15.00 - 15.15	**Eduardo Ludeña**, Escuela Superior Politecnica del Litoral, Guayaquil, Ecuador *The power series representation of the Pauli kinetic energy functional, shell structure and the Sturm-Liouville problem*
15.15 - 15.30	**Alharbi Fahhad**, Hamad bin Khalifa University, Qatar *Axiomatically Derived Kinetic Energy Density Functionals*

15.30 - 16.00 Coffee & refreshments break

Short talk Session A (parallel)
Room: Oppsittu
Chair: Karlheinz Schwarz

16.00 - 16.10 **Hualei Zhang**, Xi'an Jiaotong University, China
Ab initio investigation on high-entropy alloys

16.10 - 16.20 **He Huang**, China Academy of Engineering Physics, Jiangyou, China
Phase stability of CrCoNi ME alloys and CRSS for twinning nucleation in CrCoNi M-HE alloys

16.20 - 16.30 **Wenyue Zhao**, Beihang University, Beijing, China
Tuning the plasticity of Ni-Mo solid solution in Ni-based superalloys by ab initio calculations

16.30 - 16.40 **Noura I. Al-Zoubi**, Tafila Technical University, Jordan
First-principles study of the structural and elastic properties of Au_xV_{1-x} and Au_xNb_{1-x} alloys

16.40 - 16.50 **Danny Thonig**, Uppsala University, Sweden
Existence of Topological Nontrivial Surface States in Strained Transition Metals: W, Ta, Mo, and Nb

16.50 - 17.00 **Sergey Streltsov**, Institute of Metal Physics, Ekaterinburg, Russia
FeO_2: a possible novel magnetic constituent of Earth's lower mantle

17.00 - 17.10 **Ping Zhang**, Institute of Applied Physics and Computational Mathematics, Beijing, China
First-principles studies of plutonium oxides and their surface interaction with gaseous molecules

17.10 - 17.20 **Huilong Yu**, China Academy of Engineering Physics, Jiangyou, China
Adsorption, dissociation and diffusion of hydrogen on PuO_2 (110) surface: A DFT study

17.20 - 17.30 **Yu Yang**, Institute of Applied Physics and Computational Mathematics, Beijing, China
Structural and electronic properties of U_nO_m ($n = 1-3$,$m = 1-3n$) clusters: A theoretical study using screened hybrid density functional theory

17.30 - 17.40 **Ruizhi Qiu**, China Academy of Engineering Physics, Jiangyou, China
Orbital-free density-functional theory models for radiation damage in Al

17.40 - 17.50 **Cong Wang**, Institute of Applied Physics and Computational Physics, Beijing, China
First principle molecular dynamics studies of warm dense matter

17.50 - 18.00 **Attila Cangi**, Sandia National Laboratories, Albuquerque, USA
First-principles Stopping Power in Warm Dense Matter

Short talk Session B (parallel)
Room: Rådstuggu
Chair: David Tozer

16.00 - 16.10 **Maciej Gierada**, Cracow University of Technology, Poland
Computational Insights into Reactivity of the Supported CrO_x/SiO_2 (Phillips) Catalyst Towards Ethylene

16.10 - 16.20 **Mwombeki M. Kabanda**, North-West University, Mmabatho, South-Africa
A DFT Study on the Preferred Hydrogen Atom Transfer Pathway for the Reaction between Diethylthiourea and $^{\bullet}OH$

16.20 - 16.30 **Guilhem Javierre**, Ecole Centrale Marseille, France
Transesterification mechanism in alkyl hydrogeno-phenylphosphinates

16.30 - 16.40 **Baisheng Sa**, Fuzhou University, China
Design of Flexible Anodes for Lithium-Ion Batteries using vdW Heterostructures

16.40 - 16.50 **Robert Zaleśny**, Wroclaw University of Science and Technology, Poland
Practical hints on the selection of functionals for optical band shapes simulations: BF_2-carrying compounds as test cases

16.50 - 17.00 **Moyses Araujo**, Uppsala University, Sweden
Photocatalytic power of graphitic carbon nitride from first-principles theory: band alignment, excitonic effects and dispersive interactions

17.00 - 17.10 **Harry Ramanantoanina**, Laboratory for nuclear materials, Villigen, Switzerland
A non-empirical calculation of 2p core-electron excitation by Ligand-Field and Density Functional Theory (LFDFT)

17.10 - 17.20 **Lars Ojamäe**, Linköping University, Sweden
Computational-chemistry modelling of surface reactions and CVD growth

17.20 - 17.30 **Stephen G. Dale**, Dalhousie University, USA
Interrogating the "B05" density functional for non-locality information

17.30 - 17.40 **Mojdeh Banafsheh**, University of Geneva, Switzerland
Analytically inverted non-additive kinetic potential functional at small density overlaps

17.40 - 17.50 **Olga Lopez-Acevedo**, Aalto University, Finland
On the transferability of a parametrized kinetic functional for orbital-free density functional theory calculations

17.50 - 18.00 **Daniel Karlsson**, University of Jyväskylä, Finland
Systems with disorder, interactions, and out of equilibrium: The exact independent-particle picture from density functional theory

19.00 - 20.30 "Kräftskiva" (crayfish party/buffet) at Klockargården hotel

Friday, August 25

Contributed Session A (Parallel)
Room: Oppsittu
Chair: Per Hyldgaard

8.30 - 8.45	**Marika Savarese**, Italian Institute of Technology, Genova, Italy *Development and application of theoretical models for the characterization of complex reactions*
8.45 - 9.00	**Andreas Hansen**, University of Bonn, Germany *The new GMTKN55 database: comprehensive and state of the art benchmarking of various density functional methods including newly developed robust "high-speed" approaches*
9.00 - 9.15	**Constantin Lucian**, Italian Institute of Technology, Arnesano, Italy *Semiclassical atom theory applied to solid-state physics*

Contributed Session B (Parallel)
Room: Rådstuggu
Chair: Manuel Richter

8.30 - 8.45	**Oleg Rubel**, McMaster University, Hamilton, Canada *Electronic Localization in Semiconductor Alloys*
8.45 - 9.00	**Chiara Gattinoni**, ETH Zuerich, Switzerland *Defect chemistry and size effects in $SrRuO_3$*
9.00 - 9.15	**Menno Bokdam**, University of Vienna, Austria *Challenges and solutions for the description of hybrid perovskites with first principles methods*

Early Morning Plenary Session
Room: Oppsittu
Chair: Per Hyldgaard

9.20 - 10.00	**Eberhard Engel**, Goethe University Frankfurt am Main, Germany *Exact Exchange Plane-Wave-Pseudopotential Approach to Non-Jellium Slabs*
10.00 - 10.30	Coffee & refreshments break

Late Morning Plenary Session
Room: Oppsittu
Chair: Manuel Richter

10.30 - 10.35	Announcement of two best poster prizes
10.35 - 11.15	**Hubert Ebert**, Ludwig Maximilian University of Munich, Germany *Spin and orbital currents in magnetic solids*
11.15 - 11.20	Closing (Karlheinz Schwarz / Levente Vitos)
11.20 - 13.20	Lunch at Åkerblads gästgiveri

Posters A (Tuesday, August 22)

A1 **M. Merced Montero-Campillo**, Instituto de Quimica Medica (CSIC), Madrid, Spain
Trapping CO_2 by Adduct Formation with Azole-Based Carbenes

A2 **Fernando Steffler**, Universidade Federal de Minas Gerais UFMG, Belo Horizonte, Brasil
A TDDFT study of Keggin Polyoxometalates

A3 **Zhihua Dong**, KTH - Royal Institute of Technology, Stockholm, Sweden
Thermal spin fluctuation effect on the elastic constants of paramagnetic Fe from first-principles

A4 **Alexey Arbuznikov**, Technische Universität Berlin, Germany
On the Performance of Local Hybrid Functionals: Effects of Advanced Calibration Functions

A5 **Satoshi Yoshio**, Sumitomo Metal Minig Co., Ltd., Minato-ku, Tokyo, Japan
Analysis of optical properties of solar control materials

A6 **Stephan Schönecker**, KTH - Royal Institute of Technology, Stockholm, Sweden
Thermal surface free energy and stress of iron

A7 **Gregor Feldbauer**, Hamburg University of Technology, Germany
The acetone/TiO_2 (110) rutile hybrid interface: A DFT study on the geometry, energetics, and vibrational modes

A8 **Xiaoqing Li**, KTH - Royal Institute of Technology, Stockholm, Sweden
Anomalous ideal tensile strength of ferromagnetic Fe and Fe-rich alloys

A9 **Johannes Gugler**, Vienna University of Technology, Austria
Ab initio calculation of spin lattice relaxation of NV^- centers in diamond

A10 **Xiaojie Li**, KTH - Royal Institute of Technology, Stockholm, Sweden
Ab initio calculations of mechanical properties of reduced activation steels

A11 **Silvan Kretschmer**, Helmholtz-Zentrum Dresden-Rossendorf, Germany
Structural transformations in two-dimensional transition-metal dichalcogenide MoS_2 under electron beam: insights from first-principles calculations

A12 **Elizabeth Decolvenaere**, University of California, Santa Barbara, USA
Improving DFT for Transition Metal Alloys: The V/DM-17 Test Set

A13 **Kane Shenton**, University College London, UK
Effects of the Hubbard U on density functional-based predictions of $BiFeO_3$ properties

A14 **Ruiwen Xie**, KTH - Royal Institute of Technology, Stockholm, Sweden
Generalized stacking fault energy of C-alloyed γ-Fe: A study at paramagnetic state

A15 **Mikael Valter**, Chalmers University of Technology, Gothenburg, Sweden
Electrochemical dehydrogenation of glycerol and metanol on Au(111) with DFT

A16 **Kemoabetswe R. N. Serobatse**, North-West University, Mmabatho, South-Africa
A DFT Study on the Reaction between Thiourea and $^{\bullet}OH$

A17 **Ondrej Sipr**, University of West Bohemia, Plzen, Czech Republic
Importance of Madelung potential for magnetism of alloys: FePt studied via CPA and via supercells

A18 **Jose Garcia de la Vega**, Universidad Autonoma de Madrid, Spain
Performance of SIE and Dispersion in DFT Calculations Involving Ionic Liquids

A19 **Adam Arvidsson**, Chalmers tekniska högskola, Gothenburg, Sweden
Investigating metal dimer sites in ZSM-5 zeolites with electronic structure calculations and micro-kinetic modelling

A20 **Franca Maria Floris**, University of Pisa, Italy
Shannon entropy and correlation energy for electrons in atoms

A21 **Peter Fletcher**, Lancaster University, UK
Quantifying the Accuracy of Molecular Excited State Emission Calculated with TDDFT

A22 **Amina Mirsakiyeva**, KTH - Royal Institute of Technology, Stockholm, Sweden
The geometrical and optical investigations of PEDOT and its selenium and tellurium derivatives from the density functional theory perspective

A23 **Alexander Zech**, University of Geneva, Switzerland
A Reliability Parameter for FDET Calculations

A24 **Giovanni Lani**, Université Pierre et Marie Curie, Paris, France
Spatial and temporal non-locality in approximate exchange-correlation kernels for TDDFT

Posters B (Wednesday, August 23)

B1 **Matija Zlatar**, University of Belgrade, Serbia
Rational Design of Single Molecule Magnets — Density Functional Perspective

B2 **Attila Szilva**, Uppsala University, Sweden
Theory of non-collinear interactions beyond Heisenberg exchange; applications to bcc Fe

B3 **Jakob Seibert**, University of Bonn, Germany
Thermochromism of Ferrocene

B4 **Iulia E. Brumboiu**, KTH - Royal Institute of Technology, Stockholm, Sweden
The Electronic Structure of CoPc from an Optimally Tuned Range-Separated Hybrid Functional

B5 **Alexander Romanov**, Lobachevsky State University of Nizhny Novgorod, Russia
Time-dependent density functional theory applied to calculation of electron current excited during atom ionization by intense two-color laser pulses

B6 **Marie Humbert-Droz**, University of Geneva, Switzerland
Modelling the π conjugation length in aromatic antenna: A simple predictive tool for the synthesis of functional material

B7 **Cláudio M. Lousada**, KTH - Royal Institute of Technology, Stockholm, Sweden
Adsorption of oxygen onto aluminum — Performance of the density functionals: PBE, PBE0, M06, and M06-L

B8 **Yasmine S. Al-Hamdani**, University of Luxembourg, Luxembourg
Properties of the water to boron nitride interaction: from zero to two dimensions with benchmark accuracy

B9 **Joel Davidsson**, Linköping University , Sweden
High-thoughput search for defects in SiC

B10 **Cairedine Kalai**, UPMC, Paris, France
Combining Density-functional Theory And Wave-function Methods: The RSλH + MP2 Scheme

B11 **Simone Marocchi**, Universidade de São Paulo, Brasil
Quantum mechanics in metric space: distances between exchange-only correlations

B12 **Shuo Huang**, KTH - Royal Institute of Technology, Stockholm, Sweden
Thermal expansion in FeCrCoNiGa high-entropy alloy from theory and experiment

B13 **Szymon Śmiga**, Nicolaus Copernicus University, Torun, Poland
Accurate Kohn-Sham Ionization Potentials from Scaled-Opposite-Spin Second-Order Optimized Effective Potential Methods

B14 **Zongwei Ji**, KTH - Royal Institute of Technology, Stockholm, Sweden
Plastic deformation modes in lamellar TiAl alloys beyond the Schmid's law

B15 **Yoshifumi Nishimura**, Research Institute for Science and Engineering, Tokyo, Japan
A linear-scaling approximate DFT method for quantum mechanical molecular dynamics simulations of large systems

B16 **Giane B. Damas**, Uppsala University, Sweden
Electrochemical Reduction of Carbon Dioxide in Sn-based Electrodes: A mechanistic study

B17 **Bastien Casier**, LCPMR UMR, Paris, France
Study of the Keto-Enol Tautomerism in Acetylacetone, in Gas Phase and in Solvent

B18 **Henrik Levämäki**, University of Turku, Finland
The Becke Fuzzy Cells Integration Scheme for Exchange-Correlation in GPAW Density Functional Program

B19 **Marjan Abbasipour**, Iran University of Science and Technology, Tehran
Modification of Material Surface by plasma

B20 **Liyun Tian**, KTH - Royal Institute of Technology, Stockholm, Sweden
Density functional theory study of the formation energies of Cu-Au system

B21 **Mayura TalwelkarShimp**, Luleå Tekniska Universitet, Sweden
Some Hydrated Molecular Complexes of 4-Cyanophenylboronic acid: Significance of Water in the Structure Stabilization by Theoretical Investigations

B22 **Henry Chermette**, Universté Lyon1, Villeurbanne, France
First helical Zn(II) complex based on N4-Schiff base: Experimental and theoretical approach

B23 **Song Lu**, KTH - Royal Institute of Technology, Stockholm, Sweden
First-principles study of the semicoherent interface between TiC and Fe