TAming COmplexity in Materials Modeling (TACO)

Kick-off Meeting Program

Date: September 27 & 28, 2021

Place: Technische Universität Wien, Gußhausstraße 25-29, 1040 Vienna, Lecture Hall EI 9

Monday, September 27

12:00 – 13:00	Arrival, Get Together
13:00 – 13:15	Welcome addresses by Ulrike Diebold (TACO coordinator) and Johannes Fröhlich (Vice-Rector for Research, TU Wien)
13:15 – 13:55	Bjørk Hammer, Aarhus University Keynote l*: Machine Learning Enhanced Evolutionary Search for Structure*
13:55 – 14:25	Jesús Carrete Montaña, TU Wien (P09) *Machine-Learning Methods for Structure Prediction of Multi-Component Perovskites*
14:25 – 15:00	Coffe Break
15:00 – 15:30	Michele Riva, TU Wien (P02) *Perovskite Oxide Surfaces: Challenges and Opportunities*
15:30 – 16:00	Michele Reticcioli, University of Vienna (P07) *Polarons in TACO: Properties, Effects, and Promising Novel Recipes*
16:00 – 16:30	Aleix Comas-Vives, Universitat Autònoma de Barcelona *Tackling the Understanding of Heterogeneous Catalysts using Theory*
16:30 – 18:30	Poster Session
18:30 – Open End	Reception & Poster Viewing

Be aware that during the meeting the corona measures of the TU Wien will be enforced, which includes an **urgent appeal to get vaccinated**.

Tuesday, September 28

09:00 – 09:40	Stefan Freunberger, IST Austria Keynote II: *Reaction Mechanisms and Phase Evolution in Main Group Redox Chemistries*
09:40 – 10:10	Günther Rupprechter, TU Wien (P08) *Catalysis by Ultrathin $LaBO_3$ (B=Co, Fe) Perovskite Films: Progress Report*
10:10 – 10:40	Coffee Break & Poster Viewing
10:40 – 11:10	Andreas Nenning, TU Wien *Kinetics and Defect Chemistry of Mixed Conducting SOFC Electrodes at High Temperature*
11:10 – 11:40	Karin Föttinger & Christoph Rameshan, TU Wien (P10) *First Insights into the Structure and Reactivity of Ferrite and Perovskite Nanoparticles*
11:40 – 12:10	Gareth Parkinson, TU Wien (P04) *Water-Gas Shift Chemistry on Fe_3O_4*
12:10 – 13:40	Lunch Break
13:40 – 14:20	Anatole von Lilienfeld, University of Vienna Keynote III: *Quantum Machine Learning in Chemical Compound Space*
14:20 – 14:50	Christoph Dellago, University of Vienna (P12) *Machine Learning for Molecular Simulation: Some Successes, Challenges and Promises*
14:50 – 15:20	Coffee Break & Poster Viewing
15:20 – 15:50	Andreas Grüneis, TU Wien *Reaching Chemical Accuracy in ab initio Simulations of Complex Materials*
15:50 – 16:20	Carla Verdi, University of Vienna (P03) *Thermodynamic Properties of Zirconia from Machine Learning within and beyond DFT*
16:20 – 16:45	Final Discussion

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