

SCS Fall Meeting 2022

September 8, 2022 – 08.30-18.30h
Irchel Campus, University of Zurich



Computational Chemistry – G85

Morning Session, Chair: Prof. Jeremy Richardson

- 10:45 Fluctuations Beyond Chemical Imagination in Liquid Water [CC-011]
Ali Hassanali, The International Center for Theoretical Physics (ICTP), Trieste
- 11:15 Enzeptional: enzyme optimization via a generative language modeling-based evolutionary algorithm [CC-013]
Yves Gaetan Nana Teukam, Eindhoven University of Technology
- 11:30 Predicting chemical toxicity through machine learning [CC-014]
Christoph Schür, Eawag, Dübendorf
- 11:45 The Spectrum of Approximated Hamiltonian Matrices Representations (SPA^HM) [CC-015]
Ksenia Briling, EPFL Lausanne
- 12:00 Mechanistic investigations at the alumina/water interface [CC-017]
Carine Michel, École Normale Supérieure of Lyon

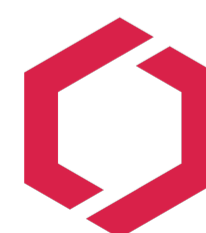
Afternoon Session, Chair: Prof. Jürg Hutter

- 14:30 Digital Chemistry at Syngenta: from academic labs to industrial applications [CC-021]
Arndt Finkelmann, Syngenta Crop Protection
- 15:00 Pathfinder - A Route Planner for Chemical Reaction Networks [CC-023]
Paul Lorenz Türtscher, ETH Zurich
- 15:15 Random projections in computational quantum mechanics [CC-024]
Aleksandros Sobczyk, IBM Research
- 15:30 Search for long-lasting electronic coherence using on-the-fly *ab initio* semiclassical dynamics [CC-025]
Alan Scheidegger, EPFL Lausanne
- 15:45 Recent Advances in the Development of Accurate Forcefields for Modelling Phase Stabilities in Hybrid Halide Perovskites [CC-026]
Mathias Dankl, EPFL Lausanne
- 16:00 Copper-Based Catalysts for CO_x Hydrogenation To Methanol – Metadynamics Bridges the Pressure and Material Gap [CC-027]
Andreas Müller, ETH Zurich



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