## Seminar of the Charles University Excellence Centre UNCE/SCI/014

Wednesday, June 23, 2022 at 13:00 in the Library of Chemistry Section, Faculty of Science

13:00-13:15

Lukáš Grajciar: Reactive neural network potentials for zeolites with DFT accuracy

13:15-13:30

**Christopher James Heard:** New directions in the modelling of encapsulated metal particles

13:30-13:45

**Dominika Zákutná**: Unravelling the magnetic and chemical morphologies of nanospheres

13:45-14:00

Lukáš Rýček: Synthesis and structure revision of natural products selagibenzophenone A and B

14:00-14:15

**Pratap Ramling Jagtap:** Synthesis of fused 1,2-naphthoquinones using a one-pot three-step reaction

14:15-14:30

Martin Zábranský: Palladium complexes of ferrocene phosphinosulfonates

14:30-14:45

**Eliška Nováková:** Generation of volatile species: Focusing on transition metals cadmium and zinc

14:45-15:00

**Kinga Golabek**: *In situ* FT-IR studies on formation of H-bonded alcohol adducts and their role in the mechanism of cyclopentanol etherification

15:00-15:15

Martin Kamlar: Enantioselective PCCP Brønsted acid catalyzed aminalization of aldehydes

15:15-15:30

**Oleg Rud**: Phase transition in hydrophobic weak polyelectrolyte gel utilized for water desalination. A computer simulation study.