



## UCT&IOCB Theoretical Chemistry Seminars

University of Chemistry and Technology, Prague, Department of Physical Chemistry

Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences

Seminars will be held in the **Seminar room B.4.29 (4th floor of the building B "Květák" of IOCB)**

or in the **Seminar room B2319 (1st floor, back entrance, building B of UCT)** on **Fridays, 14.30h.**

### Program – Spring 2026:

<b>13.2.</b>	<b>(I)</b>	<b><u>Vojtěch Košťál (IOCB):</u></b> <i>Bayesian learning for accurate and robust biomolecular force fields</i> contact: Pavel Jungwirth
<b>6.3.</b>	<b>(U)</b>	<b><u>Alexandr Malijevský (ÚCHP, UCT):</u></b> <i>Geometry-induced phase transitions in confined fluids</i> contact: Jan Heyda
<b>20.3.</b>	<b>(U)</b>	<b><u>Tomáš Ovad (UCT):</u></b> <i>Make electrons classical again: How far can we go?</i> contact: Petr Slavíček
<b>27.3.</b>	<b>(I)</b>	<b><u>Jan Řezáč (IOCB):</u></b> <i>Quantum chemistry on AI-generated structures of protein-ligand complexes</i> contact: Luboš Rulíšek
<b>10.4.</b>	<b>(I)</b>	<b><u>Stefan Grimme (Theoretical Chem., Universität Bonn):</u></b> <i>Development, Parameterization and Validation of g-xTB for Semi-empirical Quantum Chemistry Across the Periodic Table</i> contact: Luboš Rulíšek
<b>24.4.</b>	<b>(U)</b>	<b><u>Petr Kovaříček (UCT):</u></b> <i>Chemical soups cookbook: from reversible bonds, to shining light on them, to phase interfaces</i> contact: Petr Slavíček
<b>15.5.</b>	<b>(I)</b>	<b><u>Andreas Klamt (Inst. of Phys. and Theor. Chemistry, Uni. Regensburg):</u></b> <i>COSMOplex: A most efficient pathway from quantum chemistry to the thermodynamics of interfaces and microemulsions</i> contact: Luboš Rulíšek
<b>22.5.</b>	<b>(I)</b>	<b><u>Stephen Bradforth (University of Southern California, Department of Chemistry):</u></b> <i>Comparing excited state dynamics in bulk aqueous solution and at the water interface</i> contact: Pavel Jungwirth
<b>12.6.</b>	<b>(I)</b>	<b><u>Ján Michael Kormaník (IOCB):</u></b> <i>Design of catalytic metallopeptides</i> contact: Luboš Rulíšek

**I** - Seminar room **B.4.29** (4th floor of the building B "Květák" of IOCB), **Friday 14.30**

**U** - Seminar room **B2319** (1st floor, back entrance, **building B** of UCT), **Friday 14.30**