# 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** (uppermost floor of the building B "Květák" of IOCB) or in the **Conference room of FChE A402** (4th floor, building A of UCT) typically on **Fridays, 14.30h**.

## Program – Spring 2020:

<table>
<thead>
<tr>
<th>Date</th>
<th>Type</th>
<th>Speaker (Institution)</th>
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| 28.2  | (I)  | Christian Johannessen (Univ. Antwerp) | Raman optical activity of proteins: Does it even work?  
contact: Hector Martinez-Seara Monné | **Seminar room B.4.29** (uppermost floor of the building B "Květák" of IOCB), **Friday 14.30** |
| 6.3   | (I)  | Vera Krewald (TU Darmstadt) | Orbital entanglement measures for the analysis of magnetically coupled transition metal complexes  
contact: Luboš Rulišek | **Conference room of FChE A402** (4th floor, building A of UCT), **Friday 14.30** |
| 20.3  | (U)  | Ctirad Červinka (UCT) | Cohesion of crystalline materials from First-Principles: From solid methanol to crystals of ionic liquids  
contact: Jan Heyda | **Rector’s conference hall A181** (1st floor, building A of UCT), **Friday 14.30** |
| 3.4   | (I)  | Vladimír Palivec (IOCB) | Obtaining 3D atomistic structure from Raman/ROA/NMR spectroscopic techniques  
contact: Pavel Jungwirth | **Conference room of FChE A402** (4th floor, building A of UCT), **Friday 14.30** |
| 17.4  | (I)  | Johan Åqvist (Uppsala Uni.) | Computer simulations of cold-adapted enzymes  
contact: Luboš Rulišek | **Conference room of FChE A402** (4th floor, building A of UCT), **Friday 14.30** |
| 24.4  | (U*) | Zdeněk Futerka (Univ. South Bohemia) | Long-range electron transport properties of redox proteins  
contact: Petr Slavíček | **Conference room of FChE A402** (4th floor, building A of UCT), **Friday 14.30** |
| 15.5  | (U)  | Milan Ončák (Univ. Innsbruck) | Photochemical modelling in the solid state and on surfaces: Cobalt ions in MgO nanocrystals  
contact: Petr Slavíček, Jan Heyda | **Conference room of FChE A402** (4th floor, building A of UCT), **Friday 14.30** |
| 29.5  | (U)  | Štěpán Sršen (UCT) | Concept of error and Machine Learning in computational chemistry  
contact: Petr Slavíček | **Conference room of FChE A402** (4th floor, building A of UCT), **Friday 14.30** |
| 12.6  | (U)  | Tomáš Kubař (KIT) | Small chemical reactions in large molecular complexes – Multi-scale simulation  
contact: Michal Kolář | **Conference room of FChE A402** (4th floor, building A of UCT), **Friday 14.30** |

Jan Heyda  
Petr Slavíček  
Pavel Jungwirth  
Lubomír Rulišek