

French-Slovak Workshop on

Hot topics in physical chemistry & chemical physics experiments and modeling

Monday 12th September 2022

Faculty of Natural Sciences, Comenius University in Bratislava, CPS⁺ conference room (B1-322)

Programme of the workshop:

Time	Speaker and affiliation	Presentation
8h30 8h40	Josef Noga FNS ¹ /CU Bratislava	<i>Welcome speech</i>
8h40 9h10	Florent Louis PC2A ² /ULille	Recent insights into atmospheric chemistry of phytosanitary products
9h10 9h30	Dávid Vrška FNS/CU Bratislava	Noncovalent interactions
9h30 9h50	Zainab Srour PC2A/ULille	Atmospheric chlorine chemistry modelling
9h50 10h10	Juraj Országh FMPI ³ /CU	EIF spectra - molecules of astrophysical interest
10h10 10h30		<i>Coffee break</i>
10h30 11h00	Ivan Černušák FNS/CU Bratislava	Catenanes from different perspectives
11h00 11h20	Nesrine Bekkal PC2A ² /ULille	Thermochemical and kinetic studies of hydrogen abstraction reactions of halogenated polycyclic aromatic hydrocarbons by H atoms
11h20 11h40	Nissrin Alharzali FNS/CU Bratislava	Reaction mechanism of the OH-initiated atmospheric degradation of 5-chlorophenol
11h40 12h10	Valérie Vallet PhLAM ⁴ /ULille	Incorporating many-body and environment effects on core and luminescence properties
12h10 12h30	Miroslav Urban FNS/CU Bratislava	Cross-linking PET by metal atoms
12h30 14h00		<i>Lunch</i>
14h00 14h30	Céline Toubin PhLAM/ULille	Molecular level modeling of aerosol particles: molecular organization and heterogeneous reactivity
14h30 15h00	Tomáš Bučko FNS/CU Bratislava	Towards effective ab-initio calculations of thermodynamic properties
15h00 15h20	Sonia Taamalli PC2A/ULille	What is the role of microhydration on the atmospheric reactivity of iodomethane?
15h20 15h40	Jan Blaško FMPI/CU Bratislava	2D EIF spectra of pyridine
15h40 16h00	Rawan Abouhaidar PhLAM/ULille	Theoretical investigation of the ozonolysis of maleic acid droplets
16h00 16h20		<i>Coffee break</i>
16h20 16h40	Olivier Montfort FNS/CU Bratislava	Water decontamination using photochemically versatile materials
16h40 17h00	Hisham Khalifeh Al Rawas PC2A/ULille	Atmospheric reactivity of tetrachlorophenols
17h00 17h30	Ivan Černušák FNS/CU Bratislava	<i>Discussion on ongoing and future collaborations</i>

¹FNS : Faculty of Natural Sciences

²PC2A: Laboratoire Physicochimie des Processus de Combustion et de l'Atmosphère

³FMPI : Faculty of Mathematics, Physics, and Informatics

⁴PhLAM: Laboratoire de Physique des Lasers, Atomes et Molécules

Organisation: Department of Physical Theoretical Chemistry, FNS CU Bratislava



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Labex CaPPA, Programme Investissement d'Avenir, Union Européenne (FEDER), I-Site



Invited institutions:

Université de Lille et CNRS



Laboratoires PC2A et PhLAM



Comenius University in Bratislava, Faculty of Mathematics, Physics and Informatics

