

1 Detailed Program

1st Day - Tuesday, June 5th, 2018		
9:00	Arrival & Registration	
10:30	Introductory Words (Jean Christophe Tremblay)	
	Session 1: Collision and ultracold processes (Chair: Foudhil Bouakline)	
10:40	Piotr Żuchowski, University of Torun	Predicting collisional properties for the systems containing cold metastable helium from the first principles
11:15	Pablo G. Jambrina, Universidad Autónoma de Madrid	Elucidation of reaction mechanisms using quantum generalized deflection functions
11:40	Padmanaban Ramanathan, Pondicherry University	Dynamics and resonances of the $H(^2S) + CH^+$ ($X^1\Sigma^+$) reaction and isotopic effects: A quantum wavepacket study
11:40	Carles Martí, Université Toulouse III - Paul Sabatier	Effects of long range interactions on reactive and inelastic scattering: the $OH+H_2$ case study
12:20	Lunch	
	Session 2: Photochemistry and photophysics (Chair: Fabian Weber)	
14:30	Graham Worth, University College London	Full quantum direct dynamics simulations of non-adiabatic photochemistry
15:05	Tatsuhiko Murakami, UNSW Canberra	Quantum molecular dynamics for multidimensional systems by basis expansion leaping multi-configuration Gaussian (BEL MCG)
15:30	Marcin Gronowski, Polish Academy of Sciences	Photoisomerisation and electronic spectroscopy of XC_3N ($X=-CH_3, -H, -I$)
15:55	Coffee Break	
	Session 3: Imaging and Strong Fields (Chair: Markus Gühr)	
16:30	Arnaud Rouzée, Max Born Institute	Probing ultrafast molecular dynamics with ultrashort XUV pulses at free electron lasers
17:05	Jolijn Onvlee, CFEL, DESY	Unraveling the ultrafast dynamics in indole and indole-water

cont. 1 st Day - Tuesday, June 5 th , 2018		
17:30	Patricia Vindel Zandbergen, Université Paul Sabatier	Non-adiabatic alignment of CH ₃ I- ⁴ He
17:55	Diskussion on Sessions 1-3	
19:00	Postersession 1	

2 nd Day - Wednesday, June 6 th , 2018		
	Session 4: Electron dynamics (Chair: Antoine Desrier)	
9:00	Axel Lorke, University of Duisburg-Essen	Micro-photoluminescence of organic dyes in a solid matrix
9:35	Elke Fasshauer, Aarhus University	Investigating the interatomic Coulombic decay process with streaking techniques
10:00	Matthias Berg, Helmholtz-Zentrum Berlin	Towards a theoretical description of the inter-particle Coulombic decay in paired metal nanoparticle - quantum dot systems
10:25	Coffee Break	
	Session 5: Electronic structure (Chair: Vera Baturo)	
11:00	George Booth, King's College London	Development of stochastic Fock-space approaches for strongly correlated molecular systems
11:35	Caterina Cocchi, Humboldt-Universität zu Berlin	Non-linear optical properties of carbon-conjugated molecules from real-time first-principles methods
12:00	Daniel J. Arismendi-Arrieta, Donostia International Physics Center	Assesment of computational approaches for describing guest-host interactions in clathrate hydrates
12:25	Diskussion on Sessions 4-5	
12:40	Lunch	
14:30	Excursions / Free Afternoon	
19:30	Conference Dinner	

3rd Day - Thursday, June 7th, 2018		
	Session 6: Photofragmentation (Chair: Basile Wurmser)	
9:00	Markus Gühr, Universität Potsdam	Electronic and geometry views of molecules
9:35	Ashwani Tiwari, Indian Institute of Science Education and Research Kolkata	Quantum dynamical insights into fragmentations of certain molecules under influence of laser pulses
10:00	Sergio Díaz-Tendero, Universidad Autonoma de Madrid	Ultrafast hydrogen migration in ionized biomolecules in the gas phase: unusual fragmentation mechanisms
10:25	Coffee Break	
	Session 7: Quantum dynamics (Chair: Michał Smiałkowski)	
11:00	Susana Gómez - Carrasco, University of Salamanca	A ring polymer molecular dynamics approach to study the transition between statistical and direct mechanisms in the $H_2+H_3^+ \rightarrow H_3^+ + H_2$ reaction
11:35	Julien Guthmuller, Gdansk University of Technology	Theoretical investigation of Herzberg-Teller effects in resonance Raman spectra
12:00	Césaire R. Fotsing Kwetche, University of Lille, CNRS	Combining quantum chemistry with classical molecular dynamics for the theoretical study of chlorine radical reactivity at the surface of a fatty acids aerosol
12:25	Diskussion on Sessions 6-7	
12:40	Lunch Break	
	Session 8: Spectroscopy and solvation (Chair: tba)	
14:30	Martina Havenith, Ruhr-Universität Bochum	It is water what matters
15:05	Giacomo Melani, Universität Potsdam	Vibrational spectroscopy and dynamics of hydroxylated α - $Al_2O_3(0001)$ surfaces with and without water
15:30	Federico Sebastiani, Ruhr University of Bochum	Water in confinement by THz spectroscopy
15:55	Coffee Break	

	Session 9: Biologically-relevant systems (Chair: Jan Götze)	
16:30	Marie-Pierre Gaigeot, Université Paris Saclay	THz spectroscopic probing of gas phase peptides & clusters: combined IR-UV ion dip experiments and DFT-MD simulations
17:05	Nuna Galamba, Faculty of Sciences of the University of Lisbon	Free energy and molecular forces underlying sickle cell hemoglobin aggregation
17:30	Jan Joswig, Freie Universität Berlin	Allosteric control of pH-sensitive Ca(II)-binding in langerin
17:55	Diskussion on Sessions 8-9	
19:00	Second Poster Session	

4th Day - Friday, June 8th, 2018		
	Session 10: Fundamental questions in quantum mechanics (Chair: tba)	
09:00	Thomas Kühne, University of Paderborn	Nuclear motion based on the exact factorization of the time-independent electron-nuclear wave function
09:35	Mateusz Borkowski, Nicolaus Copernicus University	Optical clock transitions in ultracold ytterbium molecules
10:00	Axel Schild, ETH Zürich	Time in the Born-Oppenheimer approach
10:25	Coffee Break	
	Session 11: Processes in the condensed phase (Chair: Thomas Grohmann)	
11:00	Julia Stähler, Fritz Haber Institute of the Max Planck Society	Ultrafast electron solvation dynamics and chemistry near the DMSO/Cu interface
11:35	Marco del Cueto, Universidad Autonoma de Madrid	Surface analysis with molecular diffraction techniques: fast atomic and molecular diffraction from KCl(001) at grazing incidence conditions
12:00	Gernot Fuchs, Freie Universität Berlin	Curiosities in surfaces chemistry: a short story about anomalies and enigmatic reactions
12:25	Diskussion on Sessions 10-11	
12:40	Closing Remarks	
13:00	Optional city tour and pub crawl with the organizers	