BOOK OF ABSTRACTS OF THE

3rd GENERAL MEETING OF THE

CM1405 COST ACTION

MOLIM: MOLECULES IN MOTION

April 19 – 21, 2018

Danubius Hotel Hungaria City Center

Budapest - Hungary

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CONTENTS

CONFERENCE SCHEDULE

THURSDAY, 19/04/2018		FRIDAY, 20/04/2018	
AFTERNOON		**MORNING**	
12:00 – 14:15	Registration		
Session A	**Chair: Guntram Rauhut**	**Session D**	**Chair: Sergey Yurchenko**
14:15	Attila Császár	8:30	Rui Fausto
14:25	Roman Ciuryło	8:55	Alberto García-Vela
14:50	Anouk Rijs	9:20	Wolfgang Ernst
15:15	Csaba Fábri	9:45	Sandra Gómez
15:30 – 16:00	Coffee break	10:00 – 10:30	Coffee break
Session B	**Chair: Nadja Došlić**	**Session E**	**Chair: Roberto Marquardt**
16:00	Chiara Cappelli	10:30	António Varandas
16:25	Joao Brandão	10:55	Nadja Došlić
16:50	Halima Mouhib	11:20	Henrik Kjaergaard
Session C	**Poster session**	11:45	Viktor Szalay
17:05 – 19:00	Poster presentations		
19:00 – 21:00	Dinner	12:00 – 13:30	Lunch break
		AFTERNOON	
		Session F	**Chair: Majdi Hochlaf**
		13:30	Benoît Champagne
		13:55	Alexander Alijah
		14:20	Ove Christiansen
		14:45	Felix Iacob
		15:00 – 15:30	Coffee break
		Session G 15:30 – 17:30	**Management Committee Meeting**
		18:00 – 23:00	Conference dinner

SATURDAY, 21/04/2018		SATURDAY, 21/04/2018	
MORNING		**AFTERNOON**	
Session H	**Chair: Wolfgang Ernst**	**Session J**	**Chair: Maria Pilar de Lara-Castells**
8:30	Martin Quack	13:30	Stanislav Záliš
8:55	Liudmil Antonov	13:55	Heribert Reis
9:20	Miguel Carvajal	14:20	Kaido Sillar
9:45	Tijs Karman	14:45	Sonja Grubišić
10:00 – 10:30	Coffee break	15:10 – 15:40	Coffee break
Session I	**Chair: Martin Quack**	**Session K**	**Chair: Sonia Coriani**
10:30	Magnus Gustafsson	15:40	Kestutis Aidas
10:55	María Pilar de Lara-Castells	16:05	Sergey Yurchenko
11:20	Philippe Carbonniére	16:30	Patrick Cassam-Chenaï
11:45	Tomas Hrivnák	16:55 – 17:10	Closing ceremony
12:00 – 13:30	Lunch break	17:10 –	Free evening

PROGRAM THURSDAY (APRIL 19, 2018)

AFTERNOON	
12:00 – 14:15	**Registration**
Session A	**Chair: Guntram Rauhut**
14:15-14:25	Attila Császár
14:25-14:50	Roman Ciuryło
14:50-15:15	Anouk Rijs
15:15-15:30	Csaba Fábri
15:30-16:00	Coffee break
Session B	**Chair: Nadja Došlić**
16:00-16:25	Chiara Cappelli
16:25-16:50	Joao Brandão
16:50-17:05	Halima Mouhib
Session C	**Poster session**
17:05-19:00	Poster presentations
19:00-21:00	Dinner

SESSION I

SATURDAY, APRIL 21, 10:30

CHAIR: MARTIN QUACK

Ab-initio modelling of molecular motion under confinement

María Pilar de Lara-Castells[a], Andreas W. Hauser[b], Alexander O. Mitrushchenkov[c]

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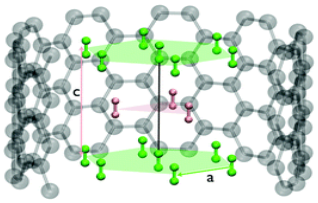
This talk is dedicated to present our ab-initio modelling of molecular motion under confinement in two different scenarios. The fundamental question addressed in the first part of my talk is if the superfluid phase existing in helium droplets is a possible liquid medium for probing a long-range electron transfer or harpoon-type reaction between heliophilic and heliophobic molecules since two antagonistic effects play an important role: On one hand, the molecular motion through the superfluid is expected to be below the critical Landau velocity, with its low value (57 m/s) favoring an electron hopping process. On the other hand, the extrusion of helium upon the entrance of the heliophobic species into the droplet is expected to add an energetic barrier to the reaction. To model it, we combine ab initio modelling in gas-phase with a concept of solvation-modified reaction pathway. The result is the presentation of clear evidences of the occurence of the harpoon-type electron transfer [1], confirming recent experimental measurements [2].

The second scenario is the inside of carbon nanotubes [3,4]. The role of quantum nuclear effects in molecular motion under confinement in carbon nanotubes is of fundamental interest, specially when dealing with light species at low temperatures. To model the system, our methodological protocol combines DFT-based symmetry-adapted perturbation theory, which we use to derive parameters for a new pairwise potential model describing the gas adsorption to the carbon material, with an adsorbate wave function-based approach characterizing accurately the quantum nuclear motion [3]. As applications, we will show how the dimensionality of molecular confinement is modified by the nanotube diameter, why a recent experiment indicates that more N_2 molecules than helium atoms are adsorbed in narrow nanotubes [5], and what ab-initio evidences are obtained for hexagonal close packing of molecular deuterium clusters (see figure, from [3]), confirming low-temperature neutron-diffraction-based experimental measurements.



[1] María Pilar de Lara-Castells, Andreas W. Hauser, and Alexander O.Mitrushchenkov, *J. Phys. Chem. Lett*. **2017**, *8*, 4284 (also see: Andreas W. Hauser & María Pilar de Lara-Castells, *Phys. Chem. Chem. Phys.* **2017**, *19*, 342).
[2] Michael Renzler et al., *J. Chem. Phys.* **2016**, *145*, 181101.
[3] Andreas W. Hauser, Alexander O. Mitrushchenkov, and María Pilar de Lara-Castells, *J. Phys. Chem. C* **2017**, *121*, 3807 (also see: Andreas W. Hauser & María Pilar de Lara-Castells, *J. Phys. Chem. Lett.* **2016**, *7*, 4929).
[4] María Pilar de Lara-Castells, Andreas W. Hauser, Alexander O. Mitrushchenkov, and R. Fernández-Perea, *Phys. Chem. Chem. Phys.* **2017**, *19*, 28621.
[5] Tomonori Ohba. *Sci. Rep.* **2016**, *6*, 28992.