ITN-EJD: Theoretical Chemistry and Computational Modelling

Second Annual Meeting, Supervisory Board Meeting and Training Workshop "Project Management Course", Leuven, Belgium, 17 – 21 July 2017. https://quantchem.kuleuven.be/ejdtccm/index.html. Local Organizers: Jeremy Harvey and Arnout Ceulemans

Program

A pdf document containing the abstracts of all oral presentations is available on the webpage. The speakers who are Early Stage Researchers within the ITN are labeled below as 'ESR' with the number of their project. All activities take place within the Maria Theresia College of KU Leuven.

Mon 17	09:30 - 12:30	*Supervisory Board Meeting**
	12:30 - 13:30	Lunch
	13:30 - 16:00	*Supervisory Board Meeting**
	16:30 - 16:35	Conference Opening
	16:35 - 17:20	**Shirin Faraji** "*Insights into light-driven DNA repair by photolyases*"
	17:20 - 17:45	**Neus Aguilera-Porta** "*In silico modelling insight into assessing NSAIDS excited states deactivation mechanisms*" ESR 8
	17:45 - 18:10	**Martina De Vetta** "*Photosensitizers for photodynamic therapy: from photophysics to assisted delivery*" ESR 7
	18:10	Welcome reception
Tue 18	09:00	Opening of Scientific Session 2
	09:00 - 09:45	**Stijn De Baerdemacker** "*When two is better than one: new wavefunctions from the seniority scheme*"
	09:45 - 10:10	**Giovanna D'Angelo** "*Knockout driven reactions in porphyrin molecules and butadiene clusters*" ESR 9
	10:10 - 10:35	**Meilani Wibowo** "*Electronic coupling calculations for a potential singlet fission chromophore*" ESR 3
	10:35 - 11:05	Coffee break
	11:05 - 11:30	**Dmytro Ivashchenko** "*Improvement of methods for the structural characterisation of drug metabolites based on collisional cross sections*" ESR 10
	11:30 - 11:55	**Enrico Skoruppa** "*DNA elasticity from coarse-grained simulations: the effect of groove asymmetry*"
	11:55 - 12:20	**Tommaso Francese** "*Magnetic fingerprint of planar bistable molecule-based magnets*" ESR 13
	12:20 - 14:00	Lunch
	14:00	Opening of Scientific Session 3
	14:00 - 14:45	**Martin Paterson** "*Development and Applications of Monte Carlo Configuration Interaction*"
	14:45 - 15:10	**Andi Cuko** "*Structure predictions of technologically and environmentally relevant oxide nanoparticles*" ESR 11
	15:10 - 15:35	**Carles Martí** "*Ab initio modelling the chemical storage of renewable energy*" ESR 4
	15:35 - 16:00	Coffee break
	16:00 - 18:00	*ESR and experts meeting + TCCM discussion**

Wed 19	09:00	Opening of Scientific Session 4
	09:00 - 09:45	**Celine Chizallet** "*Insight from ab initio calculations into the structure and reactivity of complex catalysts: the case of platinum-based subnanometric particles supported on alumina*"
	09:45 - 10:10	**Ewa Szlapa** "*Kinetics and selectivity in hydroformylation of propene*" ESR 12
	10:10 - 10:35	**Francesco Talotta** "*A theoretical investigation of the trans-[RuC(NO)(Py)$_4$]$^{2+}$ photochemistry*" ESR 6
	10:35 - 11:05	Coffee break
	11:05 - 11:30	**Stefano Battaglia** "*Electronic structure properties of [n]Cyclacenes: semi-empirical and wave function approaches*" ESR 5
	11:30 - 11:55	**Eliot Boulanger** "*Improved Lennard-Jones Parameters for Accurate Molecular Dynamics Simulations*"
	11:55 - 12:20	**Maria Izquierdo** "*Charge transfer in bulk heterojunction organic solar cells*" ESR 2
	12:20 - 15:30	Lunch + poster session
	15:30	Opening of Scientific Session 5 – in honour of Arnout Ceulemans
	15:30 - 15:40	Session opening remarks
	15:40 - 16:25	**Tohru Sato** "*Vibronic coupling density and its applications*"
	16:25 - 16:40	**Daryna Smyrnova** "*An exciting life of fluorescent proteins*"
	16:40 - 16:55	**Athanasios Arvanitidis** "*Valence bonds in elongated boron clusters*"
	16:55 - 17:40	**Patrick Fowler** "*Some current work on currents*"
	17:40 - 18:10	**Arnout Ceulemans** "*Symmetry: unquestioned answers - unanswered questions*"
	19:00	Conference Dinner
Thu 20	09:00	Opening of Scientific Session 6
	09:00 - 09:45	**Julien Michel** "*Molecular simulation methods for ensemble-based drug design*"
	09:45 - 10:10	**Gabriele dalla Torre** "*Computational approach to aluminum biochemistry*" ESR 14
	10:10 - 10:35	**Maximilian F.S.J. Menger** "*Excited state gradients in polarizable QM/MM models: an induced dipole formulation*" ESR 1
	10:35 - 11:05	Coffee break
	11:05 - 11:50	**Robert Deeth** "*Computational Coordination Chemistry: Harnessing Quantum Chemistry to Build Better Force Fields*"
	11:50 - 12:15	**Jelle Vekeman** "*Adsorption of methane on graphene*" ESR 15
	12:15 - 12:20	**Closing Remarks of the Conference**
	12:20	Lunch and end of the public sessions
	14:00	*ESR training event: Workshop "Project Management Course" - for ESRs only.* Session organizer: Berta Herrero.
Fri 21	09:00 - 12:20	*Continuation of the Project Management Course*
	12:20	*Lunch and end of the workshop*