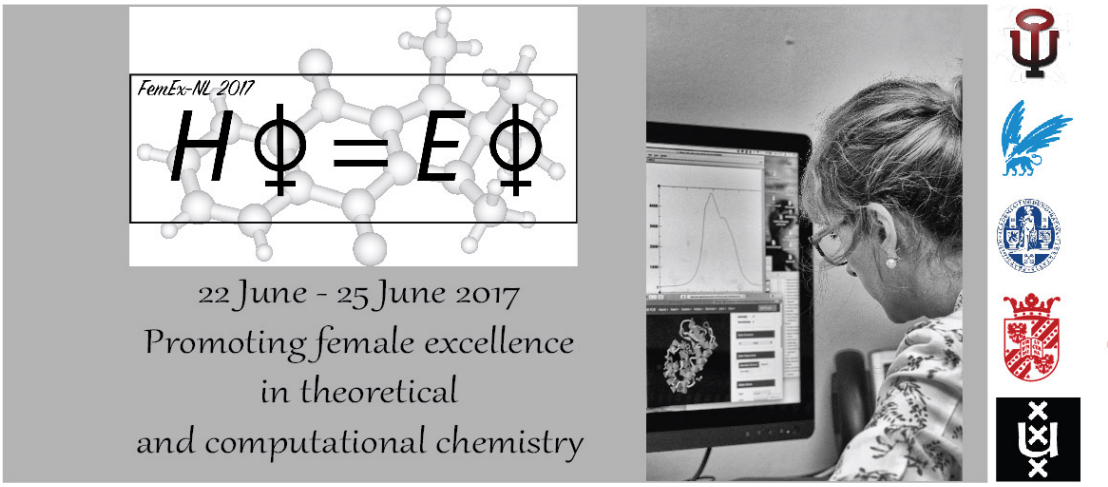

FemEx-NL 2017

Tentative Program

Thursday 22 June 2017		
14.15 – 14.30	R. Broer	Welcome
Session chair: O. Eisenstein		
14.30 – 15.10	K. Pierloot	Recent developments in multiconfigurational bio-inorganic chemistry
15.10 – 15.40	S. Harris	Mind the gap: Bridging between atomistic models and the continuum limit with fluctuating finite element analysis
15.40 – 16.10	H. Bolvin	First-principles calculations of magnetic properties of actinide complexes
16.10 – 16.40	*Coffee*	
Session chair: L. Visscher		
16.40 – 17.20	K. Coutinho	Theoretical studies of the photophysics of molecules in complex environments
17.20 – 17.50	B. Braida	1,3 dipoles: Valence bond study of their diradical character and reactivity toward alke(y)nes
17.50 – 18.20	C. Filippi	Extending the applicability of quantum Monte Carlo methods to large molecules
18.20 – 18.35	T. Lamberts	Tunneling of hydrogen transfer reactions on and in interstellar ices
18.35 – 18.50	J. de Ruiter	A closed system approach for the investigation of chemical steps involving proton and electron transfer
19.00 – 20.30	*Dinner*	
20.30 – 22.30	*Posters*	

Friday 23 June 2017		
Session chair: D. Geerke		
09.00 – 09.40	M. Swart	Spin state consistent density functionals
09.40 – 10.10	H. Cuppen	Zooming in on solid-to-solid polymorphic transitions in amino acid crystals
10.10 – 10.40	C. Domene	Studies of transport in ion channels using computer simulation
10.40 – 11.10	*Coffee*	
Session chair: K. Giesbertz		
11.10 – 11.40	S. Faraji	Insights into light-driven DNA repair by photolyases
11.40 – 12.10	J. Wu	Aromaticity-modulated noncovalent interactions
12.10 – 12.25	A. Cunha	Probing orientation of RecA on a membrane with infrared spectroscopy
12.25 – 12.40	M. Heshmat	Non-metal catalyzed H_2 splitting and hydrogenation of carbonyl compounds: Cooperation of Lewis acidity of the activated carbonyl carbon and Lewis basicity of solvent
12.40 – 14.30	*Lunch*	
Session chair: T. Helgaker		
14.30 – 15.10	M. J. Calhorda	Photophysical properties of iminopyrrolyl boron complexes: A DFT study
15.10 – 15.40	E. Dumont	Molecular dynamics investigation of DNA tandem lesions repair
15.40 – 16.10	T. van Erp	Rare event simulations reveal subtle key steps in aqueous silicate condensation
16.10 – 16.40	*Coffee*	
Session chair: E. J. Meijer		
16.40 – 17.20	K. Pernal	Intriguing van der Waals interactions revealed by electron-groups embedding approach
17.20 – 17.50	R. Bulo	New developments in adaptive QM/MM: Modeling chemistry in water
17.50 – 18.20	M. Alonso	The role of aromaticity and the π-conjugation topology in expanded porphyrins as single-molecule switches
18.20 – 18.35	O. Carstensen	Reactive molecular dynamics with ReaxFF: Complex chemical engineering processes simulated at the atomistic level
18.35 – 18.50	M. de Vetta	Thermal stability of liposome drug carriers investigated by classical molecular dynamics
19.00 – 20.30	*Dinner*	
	Session chair: B. Mennucci	
20.30 – 21.40	P. Rudolf	How to keep women (and men) in science

Saturday 24 June 2017		
Session chair: P. Gori-Giorgi		
09.00 – 09.30	H. Bahmann	Energy densities in the strong correlation limit within density functional theory
09.30 – 10.00	M. Hellgren	Correlation energy functionals based on diagrammatic many-body theory
10.00 – 10.30	B. Keller	Advanced discretization methods for Markov state models of molecular dynamics
10.30 – 11.00	*Coffee*	
Session chair: R. W. A. Havenith		
11.00 – 11.30	P. van Loosdrecht	Symmetry breaking and ultrafast processes in skyrmionic materials
11.30 – 12.00	J. Meyer	Modeling heat dissipation at the nanoscale: A tale about exciting electrons and phonons...
12.00 – 12.15	D. Lesnicki	Understanding water relaxation at interfaces
12.15 – 12.30	P. Sanchez-Murcia	Theoretical study of the photochemical properties of polypyridyl Ru(II) complexes at the interface solution/lipid membrane
12.30 – 14.00	*Lunch*	
Session chair: F. M. Bickelhaupt		
14.00 – 14.40	O. Mo	Beryllium bond outstanding features: Spontaneous formation of radicals, design of anion sponges, and Be-Be one-electron bonds
14.40 – 15.10	L. Orian	200 Years of selenium: Aspects of the chemistry and biochemistry of the moon element disclosed *in silico*
15.10 – 15.25	F. de Vleeschouwer	Inverse molecular design: Exploiting substitution effects in a systematic manner
15.25 – 16.00	*Coffee*	
Session chair: J. Vreede		
16.00 – 16.30	I. Corral Pérez	Photosensitizers based on natural nucleobases derivatives: Hacking the (genetic) code
16.30 – 16.45	N. Gaston	Designing superatomic assemblies
16.45 – 19.00	*Guided walk in the forest/free time*	
19.00 – 21.30	*Conference dinner: barbecue in the woods near the hotel*	

Sunday 25 June 2017		
Session chair: F. Buda		
09.00 – 09.40	P. Rudolf	See atoms move in real time: ultrafast electron diffraction
09.40 – 10.10	C. Calzado	Electronic structure and magnetic interactions in hybrid organic-inorganic multifunctional compounds
10.10 – 10.40	S. Riniker	Replica-exchange enveloping distribution sampling (RE-EDS) to calculate relative binding free energies
10.40 – 11.10	*Coffee*	
Session chair: I. Infante		
11.10 – 11.40	A. Borschevsky	Diatomic molecules as probes for physics beyond the Standard Model: Theoretical perspective
11.40 – 12.10	C. Sousa	Spin states in Fe(II) materials
12.10 – 12.25	J. Herzfeld	Chemistry with semi-classical electrons: Reaction trajectories auto-generated by sub-atomistic force fields
12.25 – 12.40	P.W. Langhoff	On the question of atoms and bonds in molecules
12.40 – 12.50	C. Fonseca Guerra	Poster prizes
12.50 – 13.00	FEMEX team	Closure
13.00 – 14.30	*Lunch*	