Friday June 13

11:00 – 12:30		Check In & Registration
12:30 – 14:15		Lunch
14:15-14:30		Welcoming and opening of the conference (Odile Eisenstein and Benedetta Mennucci)
Session I		**Materials, surfaces & magnetism** Chair: David Balcells
14:30-15:10	PL1	A. Selloni: Photocatalysis on metal oxides: insights from quantum simulations
15:10-15:40	IN1	R. Broer: Analysis of the spin crossover mechanism in Fe(II) complexes
15:40-16:10	IN2	L.V. Moskaleva: Silver residues as a possible key to catalytic activity of nanoporous gold: a computational study
16:10-16:40		coffee-break
16:40-17:10	IN3	M.L. Bocquet: Complex metal–organic interaction probed by first principles simulations
17:10-17:40	IN4	H. Fliegl: What are magnetically induced currents good for?
17:40-18:10	IN5	T. Jacob: Modeling electrochemical systems
18:10-18:25	O1	T.R. Walsh: Investigating Peptide-Materials Adsorption Selectivity using Advanced Molecular Simulation
18:25-18:40	O2	J.B. Rommel: Embedding Methods: Improvements, Extensions, and Chemisorption of Methane on Ni(100)
19:00-20:30		Dinner
20:30-22:30		Poster session #1

Saturday June 14

Session II		**Excited states & energy/electron transfers**	Chair: Kenneth Ruud
9:00-9:40	PL2	S. Hammes-Schiffer: Proton-Coupled Electron Transfer in Catalysis and Energy Conversion	
9:40-10:10	IN6	F. Negri: Structure-property relationships from modeling electronic, optical, charge & energy transport properties of core-extended organic semiconductor	
10:10-10:40	IN7	L. Guidoni: Electrons and protons on the way to photosynthetic water splitting	
10:40-11:10		coffee-break	
11:10-11:40	IN8	C.P. Hsu: Electronic Coupling for Singlet Fission and Triplet-Triplet Annihilation	
11:40-12:10	IN9	A. Olaya-Castro: Quantum-scale vibrations and excitation energy distribution	
12:10-12:25	O3	A. Laurent: Multiscale Modeling of a New Promising Class of Fluorescent Protein	
12:25-12:40	O4	M. Malis: Unraveling Radiationless Relaxation Pathways of Electronically Excited Biological Chromophores: From Peptides in Gas Phase to Retinal in Solution	
12:40-14:30		Lunch	
Session III		**Reactivity**	Chair: Karinne Miqueu
14:30-15:10	PL3	M. R.A. Blomberg: Quantum chemical studies of metalloenzymes – some examples from bioenergetics	
15:10-15:40	IN10	N. Lopez: Understanding industrial reactions by theoretical methods	
15:40-16:10	IN11	S. C. L. Kamerlin: Probing Evolution in the Alkaline Phosphatase Superfamily	
16:10-16:40		coffee-break	
16:40-17:10	IN12	H. Gerard: Solvation, aggregation, chelation and co.: Theoretical challenges to modelling Li+ containing organometallics	
17:10-17:40	IN13	K.H. Hopmann: The Full Reaction Mechanism of Nitrile Hydratase: a Cyclic Intermediate and an Unexpected Disulfide Switch	
17:40-18:10	IN14	J. Harvey: Ab initio determination of catalysis kinetics: Successes and challenges	
18:10-18:25	O5	A. Martin-Somer: Post-transition state dynamics in gas phase chemical reactivity: bifurcations and rotational activation.	
18:25-18:40	O6	A. Eizaguirre: Simulation of Collision Induced Dissociation Experiments of Carbohydrates	
19:00-20:30		Dinner	
20:30-22:30		Poster session #2	

Sunday June 15

Session IV		**Biology & condensed phase**	Chair: Michele Cascela
9:00-9:40	PL4	U. Rothlisberger: QM/MM Simulations in Ground and Excited States	
9:40-10:10	IN15	M. J. Ramos: Quantum mechanical studies on enzymatic reaction mechanisms	
10:10-10:40	IN16	M. Sulpizi: Water interfaces: structure and vibrational spectroscopy from DFT-based molecular dynamics simulations	
10:40-11:10		coffee-break	
11:10-11:40	IN17	L. Frediani: Pushing the limits of continuum solvation in space and time	
11:40-11:55	O7	B. Stewart: Computational Studies of Conjugated Polymer Aggregates with Surfactants in Solvent Environments	
11:55-12:10	O8	D. Major: Electrostatically guided dynamics-The root of fidelity in promiscuous terpene synthase?	
12:10-12:25	O9	S. G. Aalbergsjø: Radiation induced damage in biomolecules. An ab initio molecular dynamics study on crystalline α-L-rhamnose	
12:25-12:40	O10	K. Roos: Predicting the effect of electronic variations on ligand-target binding affinity by density functional methods	
12:40-14:30		Lunch	
Session V		**Electronic structure methods**	Chair: Trygve Helgaker
14:30-15:10	PL5	C. Corminbeuf: A Walk Through Electronic Structure Challenges in the Land of Thiophene	
15:10-15:40	IN18	P. Gori-Giorgi: Strong correlation in Kohn-Sham Density Functional Theory	
15:40-16:10	IN19	S. Coriani: Old and new spectroscopies in “strong” magnetic fields: MCD, NSCD, and MCHD	
16:10-16:40		coffee-break	
16:40-17:10	IN20	T. Saue: Simulating L3 XANES spectra of actinide compounds	
17:10-17:40	IN21	M. Pecul: Circularly polarized phosphorescence of selected diketones and enones.	
17:40-17:55	O11	H. Bahman: Efficient semi-numerical implementation of local hybrid density functionals	
17:55-18:10	O12	M. Andrejic: Application of Local Coupled-Cluster Methods to Enzymatic Reactivity	
20:00		Conference Banquet	Chair: Odile Eisenstein
21:30-22:30		After dinner talk by P. Walton: Equality in Academia. Now, Sometime or Never?	

Monday June 16

Session VI		**Dynamics** Chair: Thomas B. Pedersen
9:00-9:40	PL6	N. Makri: Quantum-Classical Path Integral: A Rigorous Methodology for Condensed-Phase Dynamics
9:40-10:10	IN22	A. Boutin: To breathe or not to breathe: the behavior of flexible MOFs upon gas adsorption or external stimuli
10:10-10:40	IN23	M. P. de Lara-Catells: Towards the Helium-mediated Soft-Landing of Embedded Nano-particles on Surfaces: Insights from Ab-initio Simulations
10:40-11:10		coffee-break
11:10-11:40	IN24	S. Bonella: Quantum effects via (almost) classical trajectories: How far can we go?
11:40-12:10	IN25	M. Barbatti: Photoinduced processes in nucleic acids
12:10-12:30		Closing remarks (Odile Eisenstein and Benedetta Mennucci)
12:30-14:30		Lunch
14:30		Departure