CSTE - Computational Spectroscopy: Bridging Theory and Experiment

Sunday 9 September

13:00		Registration
14:00		Welcome address
14:15	Vincenzo Barone:	Computational Spectroscopy: State of the Art and Perspectives
16:30	Wolfgang Lubitz:	Spectroscopic and electrochemical techniques in metal biocatalysis
18:00	Gianfranco Pacchioni	The overproduction of truth. Passion, competition, and integrity in modern science
19:00	***Cocktail***	

Monday 10 September

The Machinery: Methods and Tricks

9:00	Carlo Adamo	Density functional theory and its time-dependent implementation
11:00	***coffee break***	
11:15	Giovanni Scalmani	Characterization of the ground and excited state potential energy surface at the mean field level Local and bulk electrostatic effects via electrostatic embedding and solvent models
13:15	***lunch***	
14:15	Markus Reiher	Vibrational spectroscopy
16:15	***coffee break***	
16:30	Cristina Puzzarini	Benchmarks for Computational Spectroscopy

Tuesday 11 September

9:00	Julien Bloino	Vibrational spectroscopy beyond the harmonic approximation
11:00	***coffee break***	
11:15	Julien Bloino	Vibrationally resolved electronic spectroscopy
13:15	***lunch***	
14:15	Roland Lindh	Practical issues on the use of the CASPT2/CASSCF method in modeling photochemistry: the selection and protection of an active space
16:15	***coffee break***	
16:30	Markus Reiher	An introduction to the Density Matrix Renormalization Group

Wednesday 12 September

9:15	Nadia Rega	Time dependent and 2D-spectroscopies
11:15	***coffee break***	

How to: tools & programs 1

11:45	Roland Lindh (MOLCAS)	
13:00	***lunch***	

13:00-18:00 Poster Session

17:00 ***coffee break***

Social dinner

Thursday 13 September

Beyond the molecules: Solid state and materials

Chairman: Gianfranco Pacchioni

9:00	Hajo Freund	Model catalysts at the atomic level studied by advanced experimental techniques in surface science
11:00	***coffee break***	
11:30	Marek Sierka	Computational spectroscopy of low-dimensional materials: Tools and applications
13:00	***lunch***	
14:00	Piero Ugliengo	Vibrational spectroscopies in solids and surfaces
15:30	Silvana Botti	Electronic excitations in solids with time-dependent density functional theory and Green's function methods
17:00	***coffee break***	

Friday 14 September

9:30	Martin Kaupp	Computational magnetic resonance and more
11:30	***coffee break***	

How to: tools & programs 2 (tutorials)

11:45 Marek Sierka (Turbomole)

13:15 ***lunch***

14:00 Alberto Baiardi/Giovanni Scalmani (Gaussian)

15:30 ***coffee break***

15:45 Anna Maria Ferrari (Crystal)