

	Su 24th	Mo 25th;	Tu 26th
9:00		M. Coote H. Schwarz <i>E. Derat</i>	A. Shurki G. Gryn'ova <i>H. M. Aitken</i>
10:30		Coffee	Coffee
11:00		C. Fonseca Guerra F. Duarte J. Harvey	<i>V. Labet</i> B. Braïda M. Yanez Concluding remarks
12:30	Welcome	LUNCH (Photo)	LUNCH Box
14:00 14:30	Opening J.E. Baerends <i>O. Mo</i>	M. Head-Gordon P. Su H. Nakatsuji	Free afternoon : 2 visits are proposed (c)
15:30	Coffee	Coffee	(Aix or Marseille)
16:00	S. Shaik Y. Mo Z. Chen	<i>S. van der Lubbe</i> K. Ruedenberg P. Chen	
Social		7 pm Cocktail (a)	8 pm Conference Dinner (b)

SUNDAY

- Prof Jan Evert Baerends** Why are metal surfaces good catalysts? On the role of (relief of) Pauli repulsion ...
- Prof O. Mo Alkaline-earth (Be, Mg, Ca) bonds at the origin of huge acidity enhancements
- Prof S. Shaik Oriented-External Electric Fields: New Effectors of Chemistry
- Prof. Y. Mo The Activation of CO by B₂(NHC[^]R)₂: HOMO-LUMO Swap Without Photoinduction
- Dr Z. Chen Explicit construction of diabatic state ...

MONDAY

- Prof M. Coote** Directionality and the Role of Polarization in Electrostatic Catalysis
- Prof H. Schwarz Single-atom Catalyzed Redox Reactions in the N₂O/CO Couple:
- Dr E. Derat Understanding organometallic reactivities inside cyclodextrins 20'
- Prof C. Fonseca Guerra Molecular Recognition from a Kohn-Sham Molecular Orbital Perspective ...
- Prof F. Duarte Unraveling the Role of Non-Covalent Interactions in Recognition and Catalysis
- Prof J. Harvey Empirical Valence Bond Models: Insight from Chemical Bonding Analyses
- Prof M. Head-Gordon Some recent advances in variational energy decomposition analysis
- Dr P. Su Development of energy decomposition analysis scheme for various molecular interactions
- Prof H. Nakatsuji Free Complement (FC) Theory as a General Electronic Structure Theory
- S. van der Lubbe* Understanding Hydrogen Bonds from a Kohn-Sham Molecular Orbital Perspective: Pauli Matters
- Prof K. Ruedenberg Identifying atoms and bonding interactions that are intrinsic to ab initio electronic .. wave functions
- Prof P. Chen** Bond strengths in the gas phase, in solution, and in silico: comput. chemistry and experiment ..

TUESDAY

- Prof Avital Shurki** Design - insights from VB
- Dr G. Gryn'ova Conceptual Framework of Molecular Electronics
- H. M. Aitken Towards pH-switchable selectivity in organic synthesis
- Dr V. Labet Asynchronous character of concerted mechanisms: decomposition into primitive processes
- Dr B. Braïda Ionic excited states: the Valence Bond alternative
- Prof M. Yanez Changing the intrinsic reactivity of neutral molecules through the formation of alkaline-earth bonds