Program update # 2 (changes in ***bold-italic***)

Tuesday, June 9th	
07:30-9:00	Breakfast
SESSION 3 **Progress in DFT and theoretical methods for solids and related accuracy of properties of interest to Charge Spin and Momentum Densities** chairs: Roberto Dovesi, Vladimir Tsirelson	
09:00-09:10	General introduction
09:10-09:50	***Electronic structure of species in condensed matter environment from frozen-density embedding theory based simulations (T. A. Wesolowski - Invited)***
09:50-10:10	***Parameter-free global hybrids: an efficient tool for DFT electronic structure calculations (P. Cortona)***
10:10-10:30	***Improved thermal motion description for improved density models Refinement of lattice dynamical models from periodic ab-initio calculations (A. Ø. Madsen)***
10:30-10:50	***Thermal Expansion of Solids from Ab initio Simulations and its Effect on the Electron Momentum Distribution (A. Erba)***
10:50-11:30	Coffee break
SESSION 4 **Charge Spin and Momentum Densities in the life sciences** chairs: Sine Larsen, Paul Popelier	
11:30-11:40	General introduction
11:40-12:20	***Computation of electrostatic interaction energies in biomacromolecules from a pseudoatom databank - strengths and weaknesses (P. M. Dominiak - Invited)***
12:20-12:40	***Quantum mechanical characterization of proteins with hybrid functionals: the case of the small protein crambin (R. Dovesi)***
13:00-14:00	Lunch
SESSION 4 - continued	
15:20-15:40	***Unveiling interactions of the antimalarial drug chloroquine with haeme in aqueous solutions through spectroscopic and quantum mechanical methods (L. Lo Presti)***
15:40-16:00	***Studying the Charge Density of Large Biological Systems Transferring Extremely Localized Molecular Orbitals (B. Meyer)***
16:00-16:40	***Localization-Delocalization Matrices (LDMs) and Electron Density-Weighted Adjacency Matrices (EDWAMs): A Bridge between the Quantum Theory of Atoms in Molecules and Chemical Graph Theory (C. Matta - Invited)***
16:40-17:10	Coffee break
SESSION 5 **Functional materials: insights from charge, spin and momentum densities** chairs: Georg Eickerling, Mark Spackman	
17:10-17:20	General introduction
17:20-18:00	***Spin and Momentum Densities in Heusler Alloys (S. Dugdale - Invited)***
18:00-18:20	***An Electron Momentum Density Analysis for Spin Crossover Materials (Y. Sakurai)***
18:20-18:40	***Is the rock salt structure of SnTe so simple? (M. Sist)***
18:40-19:00	***Correlation between Materials Properties and Accurate Electron Densities: Distributed Polarizabilities of Amino Acids and their Aggregates (L. H. R. dos Santos)***
20:00-21:00	Dinner
21:30-22:30	Free time for posters and discussion