SYME 1: Frontiers of Electronic Structure Theory: Many-body Effects on the Nano-scale

Time: Friday 9:30–12:15 Location: H 0105

Invited Talk SYME 1.1 Fri 9:30 H 0105

Excitations and charge transfer phenomena in C based systems — •Elisa Molinari — University of Modena and Reggio Emilia, Modena, Italy — CNR, Istituto Nanoscienze, Modena, Italy

Excitonic effects control excitations and optical spectra in graphene-based nanostructures and related polymers [1], as well as in interacting C-based molecular systems of relevance for photovoltaics [2]. I will show results from ab-initio many body perturbation theory and discuss their implications for spectroscopies and for a realistic description of ultrafast charge separation phenomena.

[1] R. Denk et al, Nat Commun 5, 4253 (2014); A. Batra et al, Chem Sci 5, 4419-4423 (2014); L. Massimi et al, J. Phys. Chem C, in press. [2] S. M. Falke et al, Science 344, 1001-1005 (2014).

Invited Talk SYME 1.2 Fri 10:00 H 0105

Towards optimal correlation factors for many-electron perturbation theories — •Andreas Grüneis — Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — Universität Wien, Vienna, Austria

Many electron perturbation theories such as the coupled-cluster method form a hierarchy of increasingly accurate approximations to the electronic ground state wave function. This presentation will overview recent progress in applying coupled-cluster methods to solids and techniques to reduce their computational cost such as explicit correlation methods [1,2]. Furthermore applications to archetypal solid state systems as well as the uniform electron gas model system will be discussed [3].

[1] G. H. Booth, A. Grüneis, G. Kresse and A. Alavi, Nature 493, 365-370 (2013).

[2] A. Grüneis, J.J. Shepherd, A. Alavi, D.P. Tew, G.H. Booth, The Journal of chemical physics 139 (8), 084112 (2013).

[3] J.J. Shepherd, A. Grüneis, Physical Review Letters 110 (22), 226401 (2013).

Invited Talk SYME 1.3 Fri 10:30 H 0105

Towards an ab-initio description of high temperature superconductivity — •Garnet Chan — Department of Chemistry, Princeton University, United States NJ08544

I will describe our continued efforts in developing ab-initio many-body theory in the condensed phase with a view to a first principles description of a cuprate phase diagram.

Coffee break

Invited Talk SYME 1.4 Fri 11:15 H 0105

Correlation effects in unconventional superconductors: from micro- to nano- and macroscales. — •Roser Valenti — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Strasse 1, 60438 Frankfurt am Main, Germany

The combination of ab initio density functional theory with dynamical mean field theory (DFT+DMFT) has been proven to be a powerful approach for describing correlation effects in solid state systems at the microscopic level. In this talk we will focus on recent progress on this method and its application to unconventional superconductors such as Fe-pnictides, organic charge-transfer salts as well as correlated Dirac metals [1,2,3]. Further, we shall discuss the manifestation of such effects at the nano- and macroscales.

[1] I. I. Mazin *et al.* Nature Communications 5, 4261 (2014)
[2] S. Backes *et al.* New J. Phys. 16, 083025 (2014)
[3] J. Ferber *et al.* Phys. Rev. B 89, 205106 (2014)

Invited Talk SYME 1.5 Fri 11:45 H 0105

Stochastic density functional and GW theories scaling linearly with system size — •Roi Baer[1], Daniel Neuhauser[2], and Eran Rabani[3] — [1]Fritz Haber Center for Molecular Dynamics, Institute of Chemistry, The Hebrew University of Jerusalem, 91904 Israel. — [2]Department of Chemistry and Biochemistry, University of California, Los Angeles Los Angeles, CA 90095-1569 USA. — [3]Department of Chemistry, University of California, Berkeley, Berkeley, CA 94720 USA.

Kohn-Sham density functional theory (KS-DFT) is formulated as a statistical theory in which the electron density is determined from an average of correlated stochastic densities in a trace formula. Method allows reliable estimates of the electronic band structure, forces on nuclei, density and moments etc. "Self-averaging" leads to sublinear scaling. An embedded fragment stochastic DFT greatly decreases statistical fluctuations. Based on stochastic DFT a GW method is developed scaling linearly with system size. We demonstrate the results on silicon nanocrystals and large water clusters. References: *Phys. Rev. Lett. 111, 106402 (2013). *Phys. Rev. Lett. 113, 076402 (2014). *J. Chem. Phys. 141, 041102 (2014).