MM 43: Computational Materials Modelling - Transport, Excitations, Time Dependence II

Time: Wednesday 16:30–17:45 Location: H24

MM 43.1 Wed 16:30 H24

On low-energy electronic excitations in the $Ti_{1-x}Al_xN$-system — •Simon Lamowski, Torsten Weissbach, and Jens Kortus — TU Bergakademie Freiberg, Institut für Theoretische Physik, Leipziger Straße 23, 09599 Freiberg, Germany

Layered structures of $Ti_{1-x}Al_xN$ were characterized by electron energy-loss spectroscopy scanned along a direction perpendicular to the interface. By means of ab initio Density Functional Theory (DFT) calculations using the full potential linearised augmented plane wave (FP-LAPW) method as implemented in the Elk code [1] we investigate structural and electronic factors which influence the EELS up to an energy-loss of 60 eV.

Further, we go beyond standard DFT by solving the Bethe-Salpeter-Equation [2] to obtain the free parameters for the long range contribution exchange - correlation kernel [3] for time dependent DFT (TDDFT). This allows to use the TDDFT with lower computational cost to calculate EELS for supercells with defects and layers.

[1] Dewhurst K, et al. Elk. Version: 1.4.22 Available from: http://elk.sourceforge.net/
[2] Salpeter EE, Bethe HA. Physical Review; 1951;84(6):1232.
[3] Botti S, et al. Physical Review B; 2005;72(12):125203.

MM 43.2 Wed 16:45 H24

Real-time evolution in solids on the attosecond time scale — Kevin Krieger, •John Kay Dewhurst, Sangeeta Sharma, and E. K. U. Gross — Max-Planck-Institut for Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

We report on the first implementation of real-time evolution in solids in an all-electron code. Starting from the Kohn-Sham ground-state, a short laser pulse is applied to the crystal in the form of a time-dependent vector potential. The subsequent time-evolution is performed by an efficient and strictly unitary algorithm using an instantaneous LDA or GGA as the TDDFT functional. This allows the investigation of time-evolution well beyond the linear-response regime. The method is then applied to several materials in order to understand phenomena such as the spin-dynamics processes in magnetic metals. We further discuss how the time-dependent Kohn-Sham equations can be coupled to Maxwell's equations and discuss strategies for developing associated functionals.

MM 43.3 Wed 17:00 H24

Robust dynamical decoupling with concatenated continuous driving — •Kay Jahnke[1], Jian-Ming Cai[2], Boris Naydenov[1], Rainer Pfeiffer[1], Liam McGuinness[1], Fedor Jelezko[1], Martin Plenio[2], and Alex Retzker[3] — [1]Institut für Quantenoptik, Uni Ulm — [2]Institut für Theoretische Physik, Uni Ulm — [3]Racah Institute of Physics, The Hebrew University of Jerusalem, Israel

The loss of coherence is one of the main obstacles for the implementation of quantum information processing. The efficiency of dynamical decoupling schemes, which have been introduced to address this problem, is limited itself by the fluctuations in the driving fields which will themselves introduce noise. We address this challenge by introducing the concept of concatenated continuous dynamical decoupling, which can overcome not only external magnetic noise but also noise due to fluctuations in driving fields. We show theoretically that this approach can achieve relaxation limited coherence times, and demonstrate experimentally that already the most basic implementation of this concept yields an order of magnitude improvement to the decoherence time for the electron spin of nitrogen vacancy centers in diamond. The proposed scheme can be applied to a wide variety of other physical systems, including trapped atoms and ions and quantum dots, and may be combined with other quantum technologies challenges such as quantum sensing and quantum information processing.

MM 43.4 Wed 17:15 H24

photo-emission spectroscopy study for the tautomeric populations of DNA and RNA nucleobases: an application of koopmans' compliant functionals. — •ngoc linh nguyen[1], giovanni borghi[1], Nicola Marzari[1], Andrea Ferretti[2], and Ismaila Dabo[3] — [1]Theory and Simulation of Materials (THEOS), Ecole Polytechnique Federale de Lausanne — [2]CNRNANO, Universie di Modena e Reggio Emilia — [3]CERMICS, Universite Paris-Est

We study the structural and photo-electron properties of five DNA and RNA nucleobases - guanine (G),adenine (A), cytosine (C), thymine (T), and uracil (U), using either Perdew-Zunger self-interaction corrections [1] to density-functional theory, or Koopmans' compliant functionals [2]. A simple method for simulating photoemission spectra of molecules is also implemented, based on a plane-wave approximation for the final states to account for the transmission matrix. Finally, the experimental photoemission spectra are modelled by summing the individual spectra of each tautomer, weighed by the Boltzmann population ratios for the tautomers. Our calculations show that Koopmans' compliant functionals provide vertical ionization energies compatible with the values computed by high-accuracy quantum chemistry methods, and spectra that are in remarkable agreement with experimental results.

[1] J. P. Perdew and Alex Zunger, Phys. Rev. B 23, 5048 (1981).
[2] I. Dabo1, A. Ferretti, N. Poilvert, Y. Li, N. Marzari, and M. Cococcioni, Phys. Rev. B 82, 115121 (2010).

MM 43.5 Wed 17:30 H24

Nuclear quantum effects in *ab initio* IR spectra of water clusters and peptides — •Mariana Rossi[1], Volker Blum[1], Carsten Baldauf[1], Michele Ceriotti[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut, Berlin, Germany — [2]University of Oxford, UK

Nuclear quantum effects (NQE) are important in biochemical-related processes (e.g., Ref. [1]), but still present a challenge for *ab initio* (AI) treatments, especially regarding dynamical quantities. We have recently implemented two features in the all-electron code FHI-aims [2], that allow for an efficient and accurate estimation of NQE from an AI perspective: (i) Generalized Langevin Equation based thermostats (GLE) [3] that can approximate NQE, and (ii) an interface to a wrapper code [4] that performs path integral (PI) ring-polymer molecular dynamics (RPMD) and centroid molecular dynamics (CMD). With these methodologies, we quantify NQE effects in IR spectra of protonated water clusters and protonated peptides. IR spectra obtained from classical AI microcanical simulations started from GLE-thermostated runs successfully approximate NQE for small protonated water clusters. However, we provide a simple physical reason why for large and floppy peptides this approximation can fail even qualitatively, making necessary the explicit inclusion of NQE. Using AI PI based methods we can also reproduce key features of the IR spectra of Zundel-like cations observed experimentally. [1] Masgrau *et al.*, Science 312, 237 (2006) [2] Blum *et al.*, CPC 180, 2175 (2009); [3] Ceriotti, Bussi, Parrinello, JCTC 6, 1170 (2010); [4] Ceriotti, More, Manolopoulos, private communication.