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CUI THE HAMBURG CENTRE FOR ULTRAFAST IMAGING

NEWSLETTER

CUI – Graduate School

No.19, December 2018

Main topics

- Graduate Days
- Research highlights

Editorial

This newsletter closes a wonderful cycle lasted for six years, where excellent scientific results as well as important milestones in the graduate education have been attained. In particular, five graduate days and five winter schools have been organised that became an essential part of the education of our PhD students and postdocs. Another era with the newly established cluster of excellence AIM will start very soon, where such educational measures will be reinforced and integrated with novel ones. We look very much forward to the next seven years and wish you all an even more productive and successful research period.

Antonio Negretti and Peter Schmelcher

Graduate Days

The first Graduate Days (GDs) of AIM will take place on March 18-21, 2019.

The scientific programme offers a very rich selection of topics with excellent lecturers: hybrid optomechanics with atoms and membranes (Prof. Philipp Treutlein, University of Basel), 2D-IR spectroscopy (Prof. Jens Bredenbeck, University of Frankfurt), density functional theory (Dr. Klaas Giesbertz, University of Amsterdam), polaron physics in ultracold atoms and solid-state physics (Dr. Richard Schmidt, Max-Planck Institute for Quantum Optics), femtochemistry and surface physics (Prof. Wilfried Wurth, Center for Free-Electron Laser Science, DESY, University of Hamburg), nanoanalytics and cellular imaging (Dr. Thomas Braun, University of Basel). Additionally, workshops on advanced programming in Matlab and Python as well as two soft-skills workshops on scientific presentations and options for funding opportunities will take place.

As usual there will be two talks in the later afternoons: The colloquium by Prof. Päivi Törmä (Aalto University), who will provide an outlook and highlight connections between quantum geometry, superconductivity, and condensation. The industry event will have as a speaker Dr. Stephan Ritter (TOPTICA, Munich), who is an application scientist on quantum technologies and will explain how to transform them in useful applications.

For further information on the GDs, please visit the CUI website.

Research highlights

AEPs: A fresh look at the surface modelling. The atomistic ab-initio modelling of semiconductor colloidal nanoparticles (NPs) with sizes encountered in most experiments remains challenging due to the large number of atoms involved, surpassing present computational capabilities. One of the possible solutions is the use of atomic effective pseudopotentials (AEPs). AEPs are analytically connected to the self-consistent pseu-

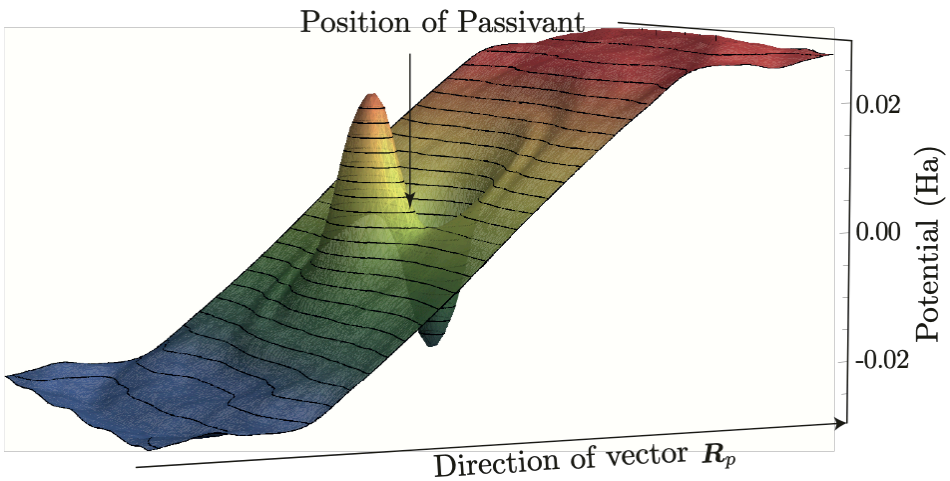

Fig. 1: Real-space potential of an isolated hydrogen atom, when only the imaginary part of the AEP is considered. The obtained surface dipole can be oriented by the vector R_p.

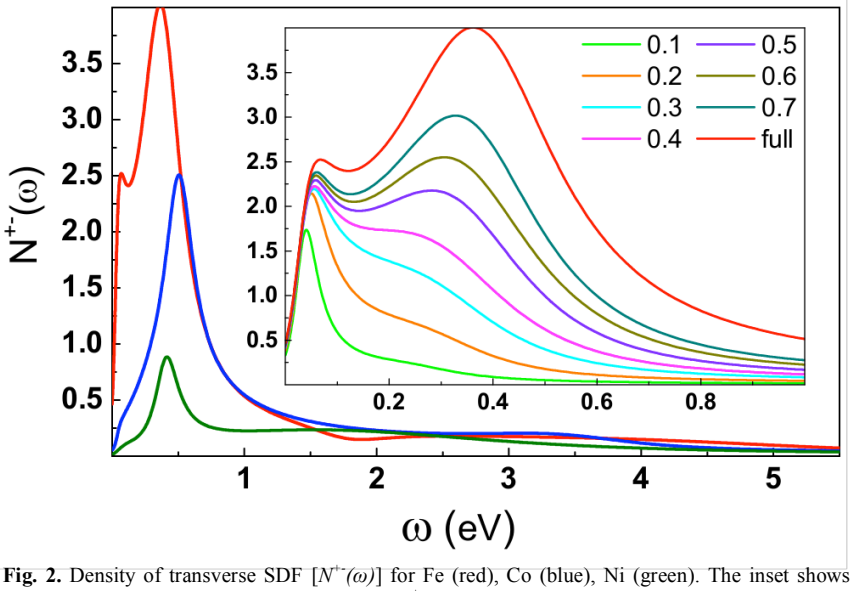

Fig. 2. Density of transverse SDF [$N^{+-}(\omega)$] for Fe (red), Co (blue), Ni (green). The inset shows the low energy part for Fe (the red curve denotes f $N^{+-}(\omega)$ for the full Brillouin zone (BZ)) compared with the density of transverse SDF evaluated in a portion of the BZ (e.g., the green line 10% of the BZ).

dopotentials from ab-initio density functional theory (DFT), but do not require the solution of a self-consistent problem and might be used to model NPs with up to 100,000 atoms. The open questions remained on how to accurately model atoms on the surface of the nanostructure, i.e. surface passivation, using the AEP methodology. The CUI PhD students Anastasia Karpulevich and Hanh Bui from the research group of Prof. Gabriel Bester have solved this problem by going beyond the conventional spherical potential approximation and have introduced an imaginary part to the AEPs (see Fig. 1). This imaginary part physically reproduces charge rearrangements naturally occurring due to surface dipoles. The pseudopotential generation uses an analytic connection to DFT and is free of parameters. The transferability of the passivation AEPs to the different sizes, types of NPs and different semiconductor materials was successfully shown. The new method opens opportunities to study surface-related optical phenomena at the atomistic level for NPs encountered experimentally.
The work has been published in Phys. Rev. B **94**, 205417 (2016).

Spin density fluctuations in ferromagnetic metals: The physics of spin density fluctuations (SDFs) in metallic magnets is very rich and complex. SDFs determine the magnetic excitation spectrum and play an important role in the magnetic dynamics. Moreover, they can strongly affect numerous static magnetic and nonmagnetic properties at zero and finite temperatures. Experimentally, SDFs are traditionally studied using the neutron scattering technique. Theoretically, SDFs in real materials can be explored from first principles by using the linear response technique based on DFT.
The CUI PhD student V. Valmispild together with CUI visitor from Ames Laboratory (USA) Dr. V. Antropov demonstrated that the SDFs are spread continuously over the entire Brillouin zone as well as the wide energy range extending far above the 3*d* bandwidth [see Phys. Rev. B **96**, 184418 (2017)]. They have shown that the on-site SDF spectrum of 3*d* ferromagnets has a generic structure that consists of two main features (see Fig. 2). One, at low energies (e.g., for Fe at ≈50 meV) is a minor contribution due to traditional low-**q** spin wave excitations, while the second, at much larger energy (e.g., for Fe at ≈0.4 eV), corresponds to large wave-vector spin excitations localised in real space.
The spin correlator, a major quantity characterizing SDF in metals, has been carefully evaluated by using the complete spectrum of SDF and the fluctuation-dissipation theorem. The related effective fluctuating moment was found to be of the order of several Bohr magnetons with a significant contribution (≈1.8μ_B) from excitations that involve semicore and high-energy states (see Fig. 3). These important results indicate that the value of the effective fluctuating moment does not depend on the presence of equilibrium local moments.

You are welcome to: ... send us suggestions of topics, which you would like to be mentioned in the next newsletter (anegrett@physnet.uni-hamburg.de).

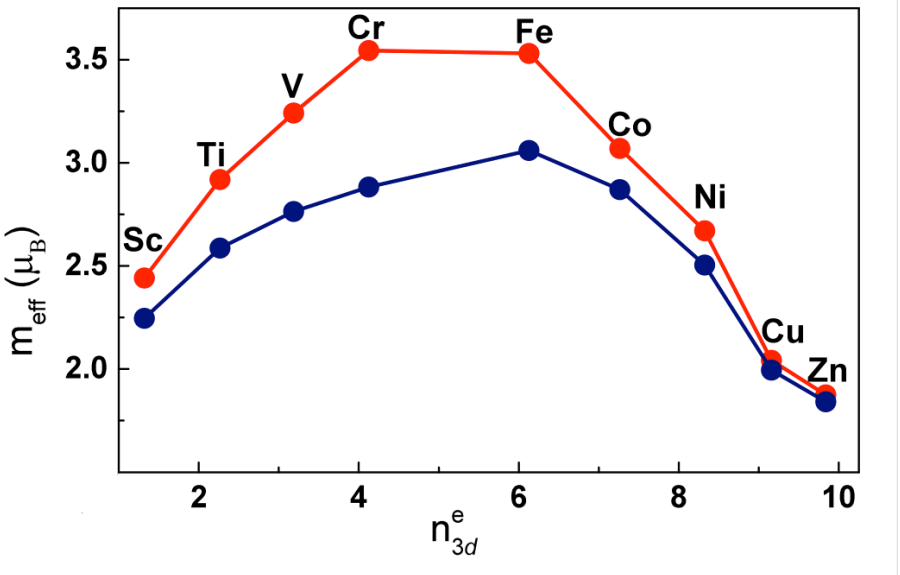

Fig. 3. The full effective fluctuating magnetic moment (m_{eff}) calculated as a function of the number of 3*d* electrons (red). The blue curve denotes not enhanced m_{eff} evaluated using the Kohn-Sham susceptibility. The effective fluctuating moment is independent of the presence of local moments and is determined solely by the 3*d* band population.