

converged molecular dynamics to room-temperature experimental data [4].

[1] V. Blum, R. Gehrke, F. Hanke, P. Havu, V. Havu, X. Ren, K. Reuter, M. Scheffler, *Comput. Phys. Commun.* **2009**, *180*, 2175-2196; <http://www.fh-berlin.mpg.de/aims/>. [2] P. Havu, V. Blum, V. Havu, P. Rinke, M. Scheffler, *Phys. Rev. B* **2010**, *82*, 161418(R). [3] A. Tkatchenko, M. Rossi, V. Blum, J. Ireta, M. Scheffler, *Phys. Rev. Lett.* **2011**, *106*, 118102. [4] M. Rossi, V. Blum, P. Kupser, G. von Helden, F. Bierau, K. Pagel, G. Meijer, M. Scheffler, *J. Phys. Chem. Lett.* **2010**, *1*, 3465-3470.

Keywords: surface, polypeptide, theory

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Optimization of materials with time dependent density functional theory

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The theory of Quantum Optimal Control (QOCT) aims to the theoretical design of external fields capable of controlling quantum mechanical systems. Nowadays, experimentally, the so-called pulse shaping techniques can be used to design pulses that produce a desired effect on atoms or molecules. These may react in complex manners when they are irradiated with high-intensity electromagnetic pulses: multi-photon, tunneling and over-the-barrier ionization, laser driven photo-induced isomerizations or fragmentations, and high harmonic generation are some of the non-linear effects that are observed.

We wish to investigate the control of these complex phenomena from first principles, by making use of time-dependent density-functional theory (TDDFT) to describe the electrons, a real-space numerical representation, and various optimization techniques.

In this talk, I will present this marriage of the QOCT techniques with TDDFT, along with various application examples.

Keywords: control, laser, theory

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Density functional calculations of electron energy loss data and inelastic mean free paths in elemental and binary materials

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Density functional theory is used to determine joint density of states and optical energy loss data for elemental metals and compounds. A novel transform algorithm is then employed to produce electron energy loss spectra and inelastic mean free paths. These results are compared with recent high profile experimental measurements in the low-energy region of strong plasmon resonances.

We present calculations of electron energy loss spectra and inelastic mean free paths determined using transformed optical loss data from density functional theory. Our novel approach enables investigation of plasmon excitation and electron scattering without the use of empirical fitting parameters or experimental data - common requirements of previous theory [1]. We consider elemental metals copper, molybdenum, zinc and selenium, and the binary semiconductor zinc selenide. The

technique is extensible to any non-crystalline or crystalline uniform material.

Results are compared with recent high precision measurements of the inelastic mean free path [2, 3] derived from x-ray absorption experiments [4, 5]. Surprising outcomes of these investigations include accurate dynamic bond lengths [6] and complementary approaches to single crystal structure [7,8]. Broadening mechanisms in the momentum-dependent energy loss function, and the energy evolution of plasmon peaks are investigated as potential sources of error in established theory. We consider the effects of crystal structure on the energy loss spectrum, and critically investigate the correlation between inelastic scattering in polyatomic systems and their corresponding elemental systems. This work focuses on electron energies below 100 eV – the region of strong plasmon resonance – where published data is highly uncertain and incomplete.

[1] S Tanuma, C.J. Powell, D.R. Penn, *Surf. Interface Anal.* **2011**, *43*, 689. [2] J.D Bourke, C.T Chantler, *Phys. Rev. Lett.* **2010**, *104*, 206601. [3] C.T. Chantler, J.D. Bourke, *J. Phys. Chem. Lett.* **2010**, *1*, 2422. [4] J.L. Glover, C.T. Chantler, Z. Barnea, N.A. Rae, C.Q. Tran, D.C. Creagh, D. Paterson, B.B. Dhal, *Phys. Rev. A* **2008**, *78*, 052902. [5] M.D. de Jonge, C.Q. Tran, C.T. Chantler, Z. Barnea, B.B. Dhal, D.J. Cookson, W.-K. Lee, A. Mashayekhi, *Phys. Rev. A*, **2005**, *71*, 032702. [6] J.L. Glover, C.T. Chantler, Z. Barnea, N.A. Rae, C.Q. Tran, *J. Physics B* **43** **2010**, *43*, 085001-1-15. [7] C.T. Chantler, C.Q. Tran, Z. Barnea, *J. Appl. Cryst.* **2010**, *43*, 64-69. [8] C.T. Chantler, *Rad. Phys. Chem.* **2010**, *79*, 117-123.

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Topological analysis of charge densities obtained from experiment and plane-wave calculations

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Accurate electron density distribution functions ($\rho(\mathbf{r})$) for crystals can be obtained from high resolution experiment and calculated by means of density functional (DFT) methods. To recover the experimental electron density one should carry out multipole refinement procedure on the dataset collected with high redundancy at low temperature. Such an “experimental” electron density function usually is suffer from systematic errors caused by thermal motion or/and absorption effects etc. Thus, DFT calculations should be “method of choice” to obtain very accurate $\rho(\mathbf{r})$ function in the case of molecular crystals. Indeed, it does not to carry out long-time experiments and multipole refinement. Unfortunately, the convergence between experimental and optimized atomic coordinates and cell parameters is still not ideal for the most of the modern DFT functionals. Besides, all-electron treatment of molecular crystals can be achieved only for small cells which are not contain heavy atoms.

The most abundant type of DFT calculations of crystals is based on the usage of plane wave basis set and pseudopotentials. Pseudopotentials are usually considered as very bad choice to obtain the $\rho(\mathbf{r})$ function suitable for the topological analysis in terms of R. Bader’s “Atoms in molecules” theory. In many cases the critical points (CP) (3,-1) could not be localized. To overcome this problem the pseudopotentials with small radius of core region (r_c) (hard pseudopotentials) should be chosen.

The suitable pseudopotentials can be generated by hand, but they are also can be obtained with quantum chemical programs. Our choice is the VASP code which is supplied with rich library of hard non-local