Structural Stability and Lattice Dynamics of Correlated Electron Materials

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How does the lattice structure of a solid depend on the correlations between the electrons? To answer this question we compute the total energy of correlated materials as a function of the atomic positions and unit cell parameters within the DFT+DMFT scheme, which combines density functional theory with the many-body dynamical mean-field theory. Results are presented for the equilibrium crystal structure and phase stability of paramagnetic Fe, in particular near the α - γ phase transition [1]. Furthermore, by combining the DFT+DMFT scheme with the method of frozen phonons the lattice dynamics and phonon dispersion relations are determined [2]. Electronic correlations are found to be essential for the explanation of the electronic and structural properties of iron.

Finally, a brief introduction into a new approach for the calculation of interatomic forces and structural distortions in strongly correlated materials is presented, which is based on the implementation of LDA+DMFT within the linear-response formalism [3]. Thereby one is able to calculate the equilibrium lattice structure of correlated systems even in the vicinity of a Mott metal-insulator transition — a computation which was not feasible up to now.

[1] I. Leonov, A. I. Poteryaev, V. I. Anisimov, and D. Vollhardt, Phys. Rev. Lett. 106, 106405 (2011).

[2] I. Leonov, A. I. Poteryaev, V. I. Anisimov, and D. Vollhardt, Phys. Rev. B 85, 020401 (2012).

[3] I. Leonov, V. I. Anisimov, and D. Vollhardt preprint arXiv:1311.4493