CFEL SCIENCE

SEMINAR

21th May 2014 - 2:00 p.m.

CFEL-bldg. 99, seminar room II

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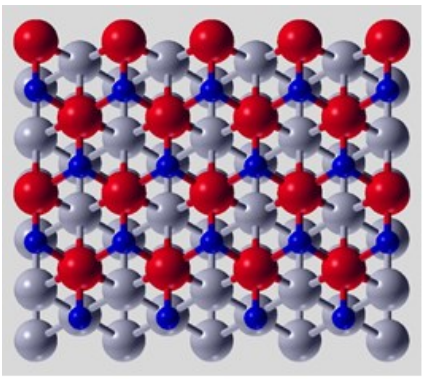
DFT studies of iron-oxide crystal and ultrathin films

FeO (wüstite) is one of the main components of the Earth's interior and the prototypical Mott insulator; its electronic band structure is determined by local electron correlations in the Fe(3d) states. A stable rock salt lattice of FeO is characterized by a high level of cation vacancies (FexO, 0.83<x<0.96). Recently, we have investigated the influence of Fe vacancies on electronic, structural and dynamical properties of FeO using the density functional theory (DFT) within the LDA+U method [1]. This study revealed a strong effect of Fe vacancies on the band structure and explained anomalous broadening of phonon spectrum observed by the nuclear inelastic scattering (NIS).

In the second part, I will present new results for ultrathin FeO layers deposited on Pt(111) surface. Oxide thin films and metal-oxide interfaces are promising systems for application in nanoelectronics, magnetic devices and catalysis. Recent progress in epitaxial growth allowed to investigate structural and dynamical properties of FeO films with thickness of one to several monolayers [2]. Significant changes in magnetic and phonon properties were observed indicating a strongly modified crystal geometry of FeO films on Pt surface. We have performed the DFT studies to investigate the electronic and lattice properties of this new FeO structure. The phonon spectrum of FeO monolayer on Pt has been obtained and compared with the NIS measurements at the ESRF.



[1] U. D. Wdowik et al., Phys. Rev. B87, 121106(R) (2013)
[2] N. Spiridis et al., Phys. Rev. B85, 075436 (2012)

Host: Robin Santra - CFEL Theory Division