European XFEL Theory Seminar

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Campus Schenefeld, main building (XHQ) room E1.096

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DFT+DMFT investigation of spin-orbit coupling assisted insulating iridates

The competition between spin-orbit coupling, crystal field splitting and electron correlations with comparable magnitude gives rise to many interesting phenomena. For instance, the so-called effective *J=1/2* state has been observed in many iridates compounds, where metal-insulator transitions occur driven by the interplay of electron correlations with magnetic ordering. Using first-principles methods, for correlated solids based on density functional theory and dynamical mean field theory (DFT+DMFT), we have investigated the metal-insulator transitions in various iridates. We explore the robustness of the effective *J=1/2* state against band effects due to itineracy, structural distortion, and strain. We show how single-particle spectra, optical conductivities, and orbital and spin moments change with strain, and we demonstrate that the ground state can be well characterized in terms of an effective energy-dependent *J=1/2* state. For the pyrochlore $RE_2Ir_2O_7$ (RE=Bi, Pr, Nd, Sm, Eu, Y) iridates compounds, the total energies obtained using charge self-consistent DFT+DMFT method reveal that the all-in-all-out magnetic ordering is stable at low temperature in late rare earth pyrochlores, while a bad metallic state is found in early rare earth pyrochlores, in agreement with experiments. We observed that the insulating pyrochlore iridates are topologically trivial, in contrast to previous theoretical predictions. At last, based on our recent calculations on $CaIrO_3$, the nature of the insulating states will be discussed based on a universal criterion.

Host:Evgeny Gorelov