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EINLADUNG zum IFP-SEMINAR

Thema: **Effect of electron-phonon interactions on orbital fluctuations in iron-based superconductors: Development and application of constrained density-functional perturbation theory**

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Host: Karsten Held

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The iron-based superconductors have attracted much attention since the discovery [1]. The pairing mechanism of the iron-based superconductors is one of the central issues and yet to be resolved. There are two strong candidates. One is the *s*-wave pairing with sign changes in the gap function (*s*±-wave) mediated by spin fluctuations [2] and the other is the *s*-wave pairing without sign changes (*s*++-wave) mediated by orbital fluctuations [3]. While the spin fluctuations are enhanced by the Coulomb repulsions, it has been recently proposed that the electron-phonon (el-ph) interactions can play a role to enhance the orbital fluctuations [3]. To examine the scenario quantitatively, it is important to derive the effective model including the phonon degrees of freedom from first principles.

In this study, we develop an *ab initio* scheme for the low-energy-model derivation of el-ph coupled system and apply it to LaFeAsO. We call the new scheme “constrained density-functional perturbation theory” [4,5], which impose a constraint on the density-response to the perturbing potential created by ionic displacements. With this constraint, the partially renormalized phonon frequencies and the partially screened el-ph interactions are estimated such that screening effects involving low-energy electrons are excluded. We analyze the resulting effective model by the random phase approximation (RPA) and show that the enhancement of the orbital fluctuations is small due to the tiny phonon-mediated exchange interactions. As a result, the spin-fluctuation-mediated *s*±-wave instability is dominant [4]. Therefore, el-ph interactions cannot be the driving force for the *s*++-wave pairing. If realized, the electron-electron vertex corrections are the driving force [6].

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