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Ab initio Low-Dimensional Physics Opened Up by Constrained RPA for Energy and Space: Applications to LaFeAsO and κ-(BEDT-TTF)$_2$X KAZUMA NAKAMURA, University of Tokyo, JST-CREST, YOSHIHIDE YOSHIMOTO, Tottori University, YOSHIRO NOHARA, MASATOSHI IMADA, University of Tokyo — Studies on outstanding electron correlation effects such as non-Fermi liquid behavior and unconventional superconductivity discovered in systems with low-dimensional anisotropy have continuously been at a front of condensed matter physics. Analyses for 1D or 2D simplified models have played a primary role in understanding essence of correlation effects, but to a large extent, the studies rely on ad hoc adjustable parameters as in the Hubbard models. We develop a new ab initio downfolding scheme for deriving effective low-energy models with low spatial dimensions [1]. The scheme is based on constrained random-phase-approximations by imposing constraints not only in "energy" but also in "space". We show real applications for 2D-layered superconductors of LaFeAsO and κ-(BEDT-TTF)$_2$X. The derived interactions in the effective models become short ranged essentially within up to next-nearest neighbors and thus justify multiband 2D Hubbard models as effective models for these materials from first principles. This work is supported from MEXT Japan under grant numbers 22740215 and 22104010.
[1] K. Nakamura, Y. Yoshimoto, Y. Nohara, and M. Imada, arXiv:1007.4429.

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