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Comparison of Ab initio Low-Energy Models for LaFePO, LaFeAsO, BaFe₂As₂, LiFeAs, FeSe, and FeTe KAZUMA NAKAMURA, University of Tokyo, JST-CREST, JST-TRIP, TAKASHI MIYAKE, AIST, JST-CREST, JST-TRIP, RYOTARO ARITA, University of Tokyo, JST-TRIP, JST-CREST, MASATOSHI IMADA, University of Tokyo, JST-CREST, JST-TRIP — We present effective low-energy models for LaFePO and LaFeAsO (1111 family), BaFe₂As₂ (122), LiFeAs (111), and FeSe and FeTe (11) [1], based on ab initio downfolding scheme, a constrained random-phase-approximation method combined with maximally localized Wannier functions. Comparison among the effective models, derived for 5 Fe-3d bands, provides a basis for interpreting physics/chemistry; material dependences of electron correlations, a multiband character entangled by the 3d orbitals, and the geometrical frustration depending on hybridizations between iron and pnictogen/chalcogen orbitals. We found that LaFePO in the 1111 family resides in the weak correlation regime, while LaFeAsO and 111/122 compounds are the intermediate region and FeSe and FeTe in the 11 family are located in the strong correlation regime. A principal parameter relevant to the physics is clarified to be the pnictogen/chalcogen height from the iron layer. Implications in low-energy properties including magnetism and superconductivity are discussed. [1] T. Miyake, K. Nakamura, R. Arita, and M. Imada, arXiv:0911.3705.

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