

Abstract Submitted
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Including many-body screening into self-consistent calculations—tight-binding model studies with Gutzwiller approximation¹ YONGXIN YAO, Iowa State University, J. SCHMALIAN TEAM, C. Z. WANG TEAM, K. M. HO TEAM — We introduce a scheme to include many-body screening process explicitly into self-consistent equations for electronic structure calculations by employing Gutzwiller approximation. The method is illustrated by applying to a tight-binding model of the strongly correlated γ -Ce. The critical Coulomb repulsion U_{ff}^c between the $4f$ electrons for electronic phase transition can be greatly raised over the usual screened value by including the main onsite many-body screening $5d$ channels. The method provides a promising way towards parameter-free *ab initio* Gutzwiller density functional theory.

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