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First-principles calculation of Hubbard parameter: Constrained local density functional approach with Maximally localized Wannier function KAZUMA NAKAMURA, Department of Physics, University of Tokyo, Japan, RYOTARO ARITA, Department of Physics, University of Tokyo, Japan, YOSHIHIDE YOSHIMOTO, Institute for Solid State Physics, University of Tokyo, Japan, SHINJI TSUNEYUKI, Department of Physics, University of Tokyo, Japan — We present a new ab initio method for calculating effective onsite Coulomb interactions of itinerant and strongly correlated electron systems. The method is based on constrained local density functional theory formulated in terms of maximally localized Wannier functions. This scheme can be implemented with any basis, and thus allows us to perform the constrained calculation with plane-wave-based electronic-structure codes. We apply the developed method to the evaluation of the onsite interaction of 3d transition-metal series. The results are discussed using a heuristic formula for screened Coulomb interactions. This work was supported by NAREGI Nanoscience Project, Ministry of Education, Culture, Sports, Science and Technology, Japan.

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