

Abstract Submitted
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First-principles calculations of magnetic transition temperatures

XIANGANG WAN, University of California, Davis , SERGEY SAVRASOV, University of California, Davis — We introduce a method to evaluate magnetic transition temperatures of strongly correlated systems. It is based on a combination of dynamical mean field theory, the local density functional theory, and employs “magnetic force theorem” for evaluating exchange constants. The method automatically predicts at a given temperature whether the system is ordered or disordered magnetically. We illustrate the approach on several systems, and discuss its accuracy in comparison with the experiment. The effect of electron-electron correlations on these predictions will be discussed.

Sergey Savrasov
University of California, Davis

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