Method for calculating the electronic structure of correlated materials from a truly first-principles LDA+U scheme

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Abstract

We present a method for calculating the electronic structure of correlated materials based on a truly *first-principles* LDA+U scheme. Recently we suggested how to calculate U from first-principles, using a method which we named constrained RPA (cRPA). The input is simply the Kohn-Sham eigenfunctions and eigenvalues obtained within the LDA. In our proposed self-consistent LDA+U scheme, we calculate the LDA+U eigenfunctions and eigenvalues and use these to extract U. The updated U is then used in the next iteration to obtain a new set of eigenfunctions and eigenvalues and the iteration is continued until convergence is achieved. The most significant result is that our numerical approach is indeed stable: it is possible to find the effective exchange and correlation interaction matrix in a *self-consistent* way, resulting in a significant improvement over the LDA results, regarding both the bandgap in NiO and the f-band exchange spin-splitting in Gd, but some discrepancies still remain.