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Removal of residual nonspherical self-interaction error in LDA+U
FEI ZHOU, VIDVUDS OZOLINS, UCLA — In the established LDA+U method, the electron self-interaction, which is generally nonspherical and orbital-dependent, is removed in a mean-field way. This results in residual self-interaction errors, particularly pronounced for f-electrons. An alternative double counting scheme that modifies the exchange, not Hartree, energy of LDA is proposed as a remedy. We show that LDA+U with our approach preserves the expected degeneracy of f^1 and f^2 states in free ions and the correct ground states in the PrO_2 solid.

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