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Locating Low-Energy Solutions within DFT+U BRYCE MEREDIG, ALEXANDER THOMPSON, CHRIS WOLVERTON, Northwestern University — The widely employed DFT+U formalism is known to give rise to many self-consistent yet energetically distinct solutions in correlated systems, which can be highly problematic for reliably predicting the thermodynamic and physical properties of such materials. While this phenomenon has been previously demonstrated for 5f compounds, we demonstrate it for 3d systems as well. We characterize the scope of these multiple energetic minima, indicating both in which systems they should occur, and the magnitude of the potential errors they introduce. We then propose an efficient method for locating the lowest-energy solution. Finally, we suggest that our method could also be extended to hybrid functionals.

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