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Towards a Density Functional Theory Exchange-Correlation Functional able to describe localization/delocalization ANN E. MATTSSON, Sandia National Laboratories, JOHN M. WILLS, Los Alamos National Laboratory — The inability to computationally describe the physics governing the properties of actinides and their alloys is the poster child of failure of existing Density Functional Theory exchange-correlation functionals. The intricate competition between localization and delocalization of the electrons, present in these materials, exposes the limitations of functionals only designed to properly describe one or the other situation. We will discuss the manifestation of this competition in real materials and propositions on how to construct a functional able to accurately describe properties of these materials. I addition we will discuss both the importance of using the Dirac equation to describe the relativistic effects in these materials, and the connection to the physics of transition metal oxides. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Ann Mattsson
Sandia National Laboratories

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