Self-Interaction Corrected Density Functional Calculations of Manganese Dimer.

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Commonly used semi-local approximations to the exchange-correlation energy in Density Functional Theory often fail to predict the correct magnetic ground state of the transition metal systems. For example, both generalised gradient approximations, such as the PBE functional, and meta-generalised gradient approximations, such as the SCAN functional, incorrectly favour the state with 3-d bounding electrons which leads to the too short bond length and the too large binding energy in Mn dimer. In this report, it is shown that this can be attributed to the spurious self-interaction error. The explicit variational self-interaction corrections to the PBE functional predict the correct magnetic ground state of the Mn dimer and restores the energy balance between antiferromagnetic and ferromagnetic states in an agreement with the experimental data and multi-configurational quantum chemistry calculations.