

Abstract Submitted
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Single-site density matrix embedding theory: from one to infinite dimensions ZHENGQIAN CHENG, CHRIS MARIANETTI, Columbia Univ — The recently developed density matrix embedding theory (DMET) has proven to be reliable for ground state properties in the Hubbard model in one and two dimensions. Here we focus on the single-site DMET, which has potential as a highly efficient method to treat actinides and oxides. We apply DMET in infinite dimensions where it can be compared to the exact solution via the dynamical mean-field theory. The results for the single band model, in addition to the two-band model with exchange and a crystal-field will be presented. Different magnetic solutions will also be presented in 1D, 2D, and infinite dimensions. We show that single-site DMET can be very reliable if one allows for magnetic solutions.

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