Abstract Submitted
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**Dynamical mean-field theory for transition metal dioxide molecules**[1] NAN LIN, DOMINIKA ZGID, Columbia University, Department of Physics, CHRIS MARIANETTI, Columbia University, Department of Applied Physics, DAVID REICHMAN, Columbia University, Department of Chemistry, ANDREW MILLIS, Columbia University, Department of Physics — The utility of the dynamical mean-field approximation in quantum chemistry is investigated in the context of transition metal dioxide molecules including $TiO_2$ and $CrO_2$. The choice of correlated orbitals and correlations to treat dynamically is discussed. The dynamical mean field solutions are compared to state of the art quantum chemical calculations. The dynamical mean-field method is found to capture about 50% of the total correlation energy, and to produce very good results for the d-level occupancies and magnetic moments. We also present the excitation spectrum in these molecules which is inaccessible in many wave-function based methods. Conceptual and technical difficulties will be outlined and discussed.

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Nan Lin
Columbia University, Department of Physics

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