Abstract Submitted
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Dynamical Mean-Field Theory for Quantum Chemistry[1] NAN LIN, Department of Physics, Columbia University, 538 West 120th Street, New York, NY 10027, USA, CHRIS MARIANETTI, Department of Applied Physics, Columbia University, New York, NY 10027, USA, ANDREW MILLIS, Department of Physics, Columbia University, 538 West 120th Street, New York, NY 10027, USA, DAVID REICHMAN, Department of Chemistry, Columbia University, 3000 Broadway, New York, NY 10027, USA — The dynamical mean-field concept of approximating an unsolvable many-body problem in terms of the solution of an auxiliary quantum impurity problem, introduced to study bulk materials with a continuous energy spectrum, is here extended to molecules, i.e. finite systems with a discrete energy spectrum. Application to chains and small clusters of hydrogen atoms yields ground state energies which are competitive with leading quantum chemical approaches at intermediate and large interatomic distances, and provides good approximations to the excitation spectrum. The method is a promising approach to the strong correlation problems of quantum chemistry.

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