

Abstract Submitted
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Cubic-scaling algorithm and self-consistent mean field for the random-phase approximation with second-order screened exchange

JONATHAN MOUSSA, Sandia National Laboratories — The random-phase approximation including second-order screened exchange (RPA+SOSEX) is an accurate model of electron correlation energy with two caveats. Its accuracy depends on an arbitrary mean field choice and its scaling of $\mathcal{O}(n^5)$ operations and $\mathcal{O}(n^3)$ memory for n electrons cannot compete with the $\mathcal{O}(n^3)$ operations and $\mathcal{O}(n^2)$ memory scaling of density functional theory (DFT). We rederive RPA+SOSEX as an approximation of the Brueckner doubles coupled-cluster (BCCD) equations, which produces a self-consistent mean field and other model corrections. In addition, we present a new algorithm for RPA+SOSEX that matches the scaling of DFT. We verify the accuracy of the new model on H_2 dissociation and the uniform electron gas and verify the reduced scaling of the new algorithm on H_n rings.

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