Abstract Submitted
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Renormalized second-oder perturbation theory for the electron correlation energy: concepts and benchmarks PATRICK RINKE, XINGUO REN, MATTHIAS SCHEFFLER, Fritz-Haber-Institute der MPG, Berlin, Germany, GUSTAVO SCUSERIA, Rice University, Houston, USA — We present a renormalized second-oder perturbation theory (R2PT) for the electron correlation energy that combines the random-phase approximation (RPA), second-order screened exchange (SOSEX) [1], and renormalized single excitations (rSE) [2]. These three terms all involve a summation of certain types of diagrams to infinite order, and can be viewed as a "renormalization" of the direct, the exchange and the single excitation (SE) term of 2nd-order Rayleigh-Schrördinger perturbation theory based on an (approximate) Kohn-Sham reference state. A preliminary version of R2PT has been benchmarked for covalently-bonded molecular systems and chemical reaction barrier heights [3] and shows an overall well balanced performance. We have extended this, by including "off-diagonal" diagrams into the rSE term and expect this refined version of R2PT to be more generally applicable to electronic systems of different bonding characteristics. Extended benchmarks of van-der-Waals-bonded molecules and crystalline solids will be presented. [1] A. Grüneis *et al.*, J. Chem. Phys. **131**, 154115 (2009). [2] X. Ren *et al.*, Phys. Rev. Lett. **106**, 153003 (2011). [3] J. Paier *et al.*, arXiv:cond-mat/1111.0173.

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