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**RPA and beyond-RPA total energy methods for strongly and weakly bonded materials**

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The random phase approximation (RPA) is attracting renewed interest as a universal and accurate method for first-principles total energy calculations. The RPA naturally accounts for long-range dispersive forces making the RPA superior to density and hybrid functionals in systems dominated by weak van der Waals or mixed covalent-dispersive interactions. We have applied the RPA to calculate the potential energy surfaces of graphene on various metal surfaces. For some of the metals, the RPA binding energy curve shows two distinct minima which arise from a delicate balance between covalent and dispersive forces that are not captured by standard semilocal or van der Waals density functionals [1]. We benchmark the RPA by calculating cohesive energies of graphite and a range of covalently bonded solids and molecules as well as the dissociation curves of H<sub>2</sub> and H<sub>2</sub><sup>+</sup>. These results show that the RPA with orbitals from the local density approximation suffers from delocalization errors and systematically underestimates covalent bond energies yielding similar or lower accuracy than the Perdew-Burke-Ernzerhof (PBE) functional for molecules and solids [1]. Inclusion of an adiabatic xc-kernel defined through a renormalization of the LDA kernel is found to significantly improve the RPA description of short range correlations yielding essentially exact results for the homogeneous electron gas [2]. By generalizing this renormalized LDA xc-kernel to inhomogeneous systems we find a fourfold improvement of RPA binding energies in both molecules and solids. We also consider examples of barrier heights in chemical reactions, molecular adsorption, and graphene interacting with metal surfaces, which are three examples where the RPA has been successful. In these cases, the renormalized kernel provides results that are of equal quality or even slightly better than the RPA, with a similar computational cost [3].

[1] T. Olsen and K. S. Thygesen, Phys. Rev. B 87, 075111 (2013)

[2] T. Olsen and K. S. Thygesen, Phys. Rev. B 88, 115131 (2013)

[3] T. Olsen and K. S. Thygesen, Phys. Rev. Lett. 112, 203001 (2014)