The random phase approximation for electron correlation: fast implementation, and application.

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The random phase approximation (RPA) for molecular correlation energies naturally includes dispersion interaction, can be applied to zero-gap systems and is non-perturbative. Despite these advantages, widespread application was hampered by its steep computational cost. Here we use resolution-of-the-identity techniques and frequency integration to reduce the scaling of RPA significantly, making applications to systems with more than 100 atoms possible. We will present timings for a Grubbs II catalyst (117 atoms). We also present results for non-covalent interactions, as well as reaction energies and barrier heights. The parameter-free RPA is an order of magnitude more accurate than (semi-)local density functionals for non-covalent interactions. For shorter ranged interactions its performance is similar to popular functionals, like B3LYP.