Open-shell Random Phase Approximation : Application to Atomisation Energies and Energy Barrier Heights

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Résumé

The Random Phase Approximation (RPA) can be derived in different variants (depending on how
the exchange interactions are handled) and in different formulations (depending on how the integrations
involved in the equations are carried out)[1]. The past explorations of the performances of these ver-
sions of RPA to calculate ground-state correlation energies of closed-shell electronic systems, in particular
systems where long-range electron-electron interaction play an important role and in the context on range-
separation[2-5], have provided a first understanding of the quality and drawbacks of these different RPAs.
Open-shell RPA has been developed and implemented for most of the variants/formulations mentioned
above. We present here tests of the use of unrestricted RPA to calculate atomisation energies and en-
ergy barrier heights. This exploration of a new range of applications gives additional insights into the
performance of the different RPA versions.

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