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Testing excited-state energy-density functionals and potentials with the ionization potential theorem MANOJ HARBOLA, HEMANADHAN MYNENI, SHAMIM MD., Indian Inst of Tech-Kanpur — The modified local spin density functional and the related local potential for excited-states are tested by employing the ionization potential theorem. The functional is constructed [1] by splitting k-space. Since its functional derivative cannot be obtained easily, the corresponding potential is given by analogy to its ground-state counterpart. Further, to calculate the highest occupied orbital energy ϵ_{max} accurately, the potential is corrected for its asymptotic behavior by employing the van Leeuwen-Barends correction [2] to it. The highest occupied orbital energy ϵ_{max} thus obtained is then compared with the ΔSCF ionization energy calculated using the excited-state functional. It is shown that the two match quite accurately, demonstrating thereby that our approach of constructing excited-state functional is on sound footing.

[1] P. Samal and M.K. Harbola, J. Phys. B: At. Mol. Opt. Phys. 39, 4065 (2006); M. Hemanadhan and M.K. Harbola, J. Mol. Struct. Theochem **943**, 152 (2010).
[2] R. van Leeuwen and E.J. Baerends, Phys. Rev. A **49**, 2421 (1994).

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