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Density functional calculation of ground and excited states of negative atoms AMLAN K. ROY, Department of Chemistry, University of Kansas, Lawrence, KS, 66045, USA — Accurate determination of negative ions pose considerable challenge in both theory and experiment. Present study extends the validity and domain of a density functional theory (DFT)-based formalism, found quite successful for a wide variety of atomic excited states, in regards to the case of ground and metastable bound excited states of atomic anions. The local work-function-based exchange and nonlocal Lee-Yang-Parr correlation potential is used, while the radial Kohn-Sham equation is solved by means of generalized pseudospectral method. A number of quantities such as total energy, radial density, density moment and transition wavelength for the anions of first and second-row atoms show reasonably good agreement with available theoretical and experimental results. For example, absolute deviation in total energy remains within 0.007-0.171% for Li^- and Be^-, while the transition wavelengths show absolute deviation of 0.891% and 0.438% relative to the experimental values. In short, this offers a simple practical route towards accurate and reliable calculation of ground and excited states of atomic negative ions.

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