

Abstract Submitted
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A DFT approach for the accurate calculation of triply excited hollow and doubly-hollow Rydberg resonances in lithium isoelectronic sequence AMLAN KUSUM ROY, Department of Chemistry and Biochemistry, University of California, Los Angeles, CA, 90095, USA — Density functional calculations are performed for the $2l2l'nl''$ ($n \geq 2$) triply excited *hollow* resonances in lithium isoelectronic sequence. An amalgamation of the local nonvariational work-function-based exchange potential and LYP correlation functional is used. Radial KS equation is solved accurately through the Generalized pseudospectral method, leading to a nonuniform and optimal spatial discretization. Results are presented on the excited-state energy, excitation energy, radial density and other expectation values. A large number of states are studied, covering low, moderately-high and high-lying excitations, with n as high as up to 25, having varied symmetries and multiplicities. Companion calculations are made for the $3l3l'nl''$ ($n \geq 3$) *doubly-hollow* states of Li in the photon energy range of 176-181 eV. Detailed comparisons with recent theoretical and experimental results show excellent agreement. Many *new* resonances are presented for the first time, which can provide useful guidelines for future studies. This provides a simple, efficient and general scheme for reliable and accurate treatment of multiply excited Rydberg resonances in atoms within DFT.

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