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Ab initio Multi-configurational Dirac-Hartree-Fock (MCDHF) calculations of the energy spectrum of neutral Lawrencium

The study of the actinides lies at the frontier of contemporary nuclear and atomic physics research. Lawrencium, with 103 protons, is the heaviest and final actinide in the periodic table, however few experimental results exist for neutral Lawrencium.

Calculations of the energy spectrum were initially performed on its lighter homologue Lutetium for which experimental results exist. Lutetium is calculated in order to determine the predictive accuracy of the calculations and suitability of the model in calculating the energy spectrum and transition properties of Lawrencium.

The energy spectra of Lawrencium and Lutetium are investigated using Multi-configurational Dirac-Hartree-Fock (MCDHF) method and the preliminary results of the latter are presented. In addition, a multireference (MR) set is built containing configuration state functions (CSFs) which significantly contribute to the reference level wavefunction.

The calculations are performed using a layer-by-layer approach. The spectroscopic orbitals in the multireference are generated in Dirac-Hartree-Fock mode without correlation. Higher layers are generated by allowing excitations from the multireference into the virtual layers.

Field

Enhancing the understanding of the actinide atomic structure

Secondary field

Call for support

No

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