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Relativistic Quantum Mechanical Calculations on Alkali Atoms and Dimers from Cesium to Ununennium CHUKWUNONSO ARINZE, WALTER ERMLER, University of Texas at San Antonio — Ab initio calculations using relativistic effective core potentials, and intermediate angular momentum coupling of electrons are carried out on the alkali metal atoms, and dimers from cesium through ununennium. A spin-orbit configuration interaction (SOCI) method is employed that includes a spin-orbit coupling operator and a relativistic effective core potential in the Schrodinger Hamiltonian operator. The energy levels from these calculation are found to reproduce the positions of the experimental spectral lines and predict lines not heretofore observed for both of these atoms.

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