PHYSICS&ASTRONOMY
THE UNIVERSITY OF TEXAS AT SAN ANTONIO

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Friday, March 31s, 2017
AET 0.204
3:15 PM

Quantum Mechanical Calculations of Spectral Properties of Heavy Element Molecules

We have developed software and databases for *ab initio* electronic structure calculations that incorporates spin-orbit coupling and other relativistic effects to study polyatomic systems comprised of heavy elements. These are employed to elucidate structures and spectra of heavy transition metal, actinide, lanthanide, and super heavy atom systems. The software module that corresponds to the scaling bottleneck in accurate wave function calculations has been implemented on advanced massively parallel processor computer architectures capable of performance in the teraflops to petaflops range. This module was developed within the Columbus suite of quantum chemistry codes. Our implementation of relativistic quantum chemical methods for massively parallel computers enables us to calculate properties of heavy-element systems at the same levels of theory currently available for light-element ones. The methodology so developed supplements current experimental studies of the actinides, lanthanides, and radioactive heavy transition metal elements, allowing limited or sparsely available experimental data to be extended and interpreted. Results of calculations of properties and spectra, including line intensities, will be presented for a variety of molecular systems including RuO^+ and OsO^+, $Pt@C_{10}$, PbO and LiSr.

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