Fully-Relativistic Linear Combinations of Gaussian Type Orbitals Electronic Structure Technique For Solids and Films*

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The linear combinations of Gaussian type orbitals (LCGTO) technique is perhaps the most widely used electronic structure technique in existence today, due to its ability to treat such diverse systems as isolated clusters of atoms, 2D periodic films, and 3D periodic solids. The range of applicability of the LCGTO method has however suffered from the lack of a stable technique for incorporating relativistic effects, due to the so-called variational collapse problem, effectively restricting LCGTO calculations to the first three rows of the periodic table. During the last decade, this obstacle has been successfully overcome by using the Douglas-Kroll-Hess transformation to generate two-component equations that are both variationally stable and computationally tractable. This talk will describe the development of the first nonperturbative, all-electron, fully-relativistic LCGTO electronic structure method for crystalline solids and 2D periodic films. A recent application of this method to the zero-pressure properties of the light-actinide metals will be discussed.

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