

Efficient Use of Basis Sets in Relativistic Molecular Calculations

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Relativistic molecular calculations are important in such areas as the development of new materials, where heavy elements play a significant role as catalysts for producing materials or as part of the material itself. Often such calculations are made on reduced models of a larger system, perhaps with environmental embedding. As relativistic calculations are usually much more demanding than nonrelativistic calculations, the efficiency of the calculations is a critical issue. This is particularly important when calculations are used in large-scale screening of enumerated structures in a search for optimal properties for a particular application.

One aspect of efficiency is the choice of appropriate basis sets for the particular type of calculation. In this presentation, an overview of different kinds of basis sets and their efficient use with various all-electron relativistic methods will be given, and some recent developments for specific methods will be discussed.