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The choice of Gaussian basis sets for molecular electronic structure calculations

Reinhart Ahlrichs and Peter R. Taylor

Institut für Physikalische Chemie und Elektrochimie, Universität Karlsruhe, Kaiserstrasse 12, 7500 Karlsruhe, Fed. Rep. Germany.

Abstract

The choice of Gaussian type basis sets for electronic structure calculations of molecules is discussed in detail for treatments on the SCF and Cl level. This article is organized in the following sections : I. Introduction, II. Mathematical foundation of the LCAO-MO method, III. Basis sets of first and second row atoms in SCF calculations, IV. Transition metals, V. Beyond-Hartree-Fock calculations, VI. Summary.

Detailed proposals are made for the choice of basis sets at various levels of computational expense.

Résumé

On discute en détail le choix des bases de type Gaussien pour le calcul de structures électroniques de molécules par traitement au niveau SCF et Cl. L'article est organisé comme suit : I. Introduction, II. Bases mathématiques de la méthode LCAO-MO, III. Ensembles de bases pour les calculs SCF sur les atomes de la première et seconde période, IV. Métaux de transition, V. Calculs au delà de Hartree-Fock, VI. Conclusions.

Propositions détaillées pour le choix d'ensembles de bases à différents niveaux de dépenses de calcul.

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