

Quantum Chemistry: The Challenge of Transition Metals and Coordination Chemistry (Nato Science Series C:)



Over the last twenty years, developments of the ab initio methodologies and of the computing capacities have progressively turned quantum chemistry into a predictive tool for molecular systems involving only light elements. The situation appears less advanced for systems containing transition metal elements where specific difficulties arise, like those linked to the quasi-degeneracy of the lowest atomic states. Correlation effects, which are important only for quantitative accuracy in the treatment of molecules made of light elements, need sometimes to be considered even for a qualitative description of transition metals systems (like the multiple metal-metal bond). The treatment of atoms of a high atomic number has necessitated the development of model potential methods. These difficulties exacerbate for systems containing several transition atoms a correct description of the dichromium molecule Cr₂ still represents a challenge to quantum chemists. Yet many advances have been made recently in the theoretical treatment of these systems, despite the fact that our understanding still remains disparate with a variety of models and methodologies used more or less successfully (one-electron models, explicitly correlated ab initio methods, density functional formalisms). For these reasons, a NATO Advanced Research Workshop was organized to review in detail the state-of-the-art techniques and at the same time the most common applications. These encompass many fields including the spectroscopy of diatomics and small aggregates, structure and reactivity problems in organometallic chemistry, the cluster surface analogy with its implications for heterogeneous catalysis and the description of extended structures.

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