EDITORIAL FOREWORD

Many electron systems possessing a limited number of degrees of freedom are now accessible for a practically exact quantum mechanical treatment within the nonrelativistic Born–Oppenheimer approximation. Such systems are free atoms or small molecules treated as independent quantum systems in vacuo, i.e. they are cut out from their natural environment. The proper treatment of environmental effects resulting from the mutual interactions of atoms and molecules, as well as the quantum chemical description of large molecules with a large number of degrees of freedom, remain a formidable task if no simplifying models are introduced.

In the last few years, it has become evident that a similar methodology can be applied to weak intersystem interactions, environmental effects, as well as to the treatment of large molecules. The most important part of an extended system can be approximately described as being embedded into the effective field of the rest of the system.

This special collection of papers provides a cross section of the above, rather general embedding problem. The concept of embedding has strong roots in solid-state physics. This collection of papers will, however, focus mainly on molecules. The ordering of the papers is naturally somewhat arbitrary, but we still wanted to follow some logic in arranging them. An exact treatment of the electronic structure of embedded molecules gives rise to serious theoretical difficulties due to the antisymmetry requirement of the Pauli principle. For interacting molecules, this problem is discussed in the first paper by Adams. A related question, the derivation of the proper effective equation for embedded molecules, fragments and clusters, is treated by the next three papers by Huzinaga et al., Seijo and Barandiarán, and Mehler. The latter work also discusses a possible solution of the problem of non-orthogonality of fragment orbitals.

The next three papers, by Ángyán, Tapia, and Miertus and Frecer, respectively, are devoted to different aspects of solvent effect theories, where the molecule under investigation is embedded in an environment represented by the solvent.

An energy partitioning scheme based on two-electron functions, geminals, is proposed for intermolecular interactions in the next paper by Røeggen.

The formalisms of the above papers were primarily elaborated for the ground state. Studying excitations, chemically well-defined chromophores can be considered as embedded units. The next two papers are devoted to excited states. Hansen and Bouman investigate molecular electronic excitations. Peluso, Adamo and Del Re provide a vibrational analysis.

The following three papers open the doors to solid-state applications. An important special case of embedding is represented by the problem of trapping molecules into rare-gas matrices. A model to treat this situation is elaborated by Silvi et al. László uses a formalism of pseudo atoms and a partitioning technique, and applies it to buckminster fullerene type structures and covalent silicon clusters, investigating

topological properties. Kürti and Surján study the role of long-range interactions between a conjugated polymer and an embedded unit cell in a specific π-electron model.

The final paper, by Arteca and Mezey, describes a topological framework for studying the conformational dependence of molecular shapes, formulated as an embedding problem of nuclei within electronic clouds.

The rich variety of possible topics of molecular embedding could fill several volumes. A complete account of the field is not at all represented by the papers of this volume. Nevertheless, this collection of papers covers a wide range of interest, from fundamental mathematical problems to chemical applications.

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