Exploiting the Transferability of Extremely Localized Molecular Orbitals to Study Large Biological Systems

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Nowadays, one of the goals of theoretical chemistry consists in developing new quantum mechanical strategies to study large molecular systems at a sensitively reduced computational cost. In this context several research groups have developed different linear scaling methods [1-3] that have been successfully used in important fields, such as molecular material modeling and drug design.

A very interesting option to address this challenge is based on the observation that molecules are generally constituted by recurrent functional groups that roughly maintain the same properties in different chemical environments. Therefore, following a sort of LEGO approach [4], one could imagine to define transferable localized Molecular Orbitals (MOs) describing the above mentioned functional units, which would allow to almost instantaneously obtain the wave function (or the electron density) of a very large system.

Unfortunately, the canonical Hartree-Fock MOs and the traditional localized MOs are completely or partially delocalized on the whole systems on which they are calculated and, therefore, they are not suitable for our purpose. Nevertheless, it is possible to resort to the concept of Extremely Localized Molecular Orbitals (ELMOS) [5] that are orbitals strictly localized on small molecular functional units and can be easily transferred [6, 7] from a molecule to another one.

Our main goal is to construct a database of ELMOs that cover all the possible functional groups of the twenty natural amino acids. To accomplish this task we have started investigating in detail the transferability of the Extremely Localized Molecular Orbitals to quite large biomolecular systems (e.g. Leu-enkephalin polypeptide). In particular, we have compared the resulting electron densities to charge distributions both calculated by means of more traditional and expensive methods, and obtained through the transfer of experimental pseudo-atoms [8], which are used to refine protein crystallographic structures.

The obtained results are in good agreement with the considered benchmarks and a general database of ELMOs is currently under construction.

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