Assessing the transferability of Extremely Localized Molecular Orbitals to large systems

Benjamin Meyer[*†1] and Alessandro Genoni[‡1]

[1]Structure et Réactivité des Systèmes Moléculaires Complexes (SRSMC) – CNRS : UMR7565, Université de Lorraine : UMR7565 – France

Résumé

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 recently developed different linear scaling methods that have been successfully used in important fields, such as molecular material modeling and drug design.

In this framework one possibility is based on the observation that molecules are generally constituted by recurrent functional units roughly maintaining the same properties in different environments. Therefore, following a sort of LEGO approach, if we could define transferable localized Molecular Orbitals (MOs) describing the above mentioned functional units, in principle we would be able to almost instantaneously obtain the wave function (or the electron density) of very large systems.

Unfortunately, the canonical Hartree-Fock MOs and the traditional localized MOs are completely or partially delocalized on the whole system on which they are calculated and they are not suitable for the purpose mentioned above. That is the reason why, in this approach, it is necessary to resort to the Extremely Localized Molecular Orbitals (ELMOS) [1] that are orbitals strictly localized on small molecular functional units and that can be easily transferred [2, 3].

Our goal is to construct a database of ELMOs that cover all the possible functional groups of the natural amino acids. To accomplish this task we are currently studying the transferability of the Extremely Localized Molecular Orbitals to quite large biomolecular systems (e.g. Leu-enkephalin polypeptide) comparing different electron densities resulting from the transfer of ELMOs defined on different set of model molecules.

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[*]Intervenant

[†]Auteur correspondant: benjamin.meyer@univ-lorraine.fr

[‡]Auteur correspondant: alessandro.genoni@univ-lorraine.fr