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Libraries of extremely localized molecular orbitals

Alessandro Genoni[1]
[1]*Laboratoire SRSMC - CNRS & University Of Lorraine, Metz, France*
E-mail: Alessandro.Genoni@univ-lorraine.fr

In spite of recent technological and methodological improvements, determining electron densities of very large systems (e.g., proteins) remains a difficult challenge. In the crystallography community this drawback has been overcome by exploiting the reliable transferability of the multipole model pseudoatoms, which can be really considered as atomic LEGO building blocks to reconstruct the charge distributions of large molecules. This observation led to the construction of different pseudoatoms databanks that have been already used to successfully refine crystallographic structures and to compute electrostatic properties of macromolecules.

Although the pseudoatoms libraries are by now well-established tools to study the charge density of very large systems, nowadays a possible alternative is represented by the use of Extremely Localized Molecular Orbitals (ELMOs) [1]. These are orbitals strictly localized on small molecular subunits (e.g., atoms, bonds, or functional groups) and, for this reason, they are also easily exportable from a molecule to another provided that the fragments on which they are localized have similar chemical environments in the original and target molecules.

In order to exploit the ELMOs transferability, in our group we have recently constructed libraries of Extremely Localized Molecular Orbitals that cover all the possible fragments of the twenty natural amino acids in all their protonation states. These databases can be considered as original quantum mechanical force fields and represent the starting point for the forthcoming developments of novel linear-scaling quantum chemical strategies to refine crystallographic structures of proteins.

In this talk, our preliminary investigations to the construction of the ELMOs databanks will be presented. In particular, a special attention will be dedicated to the studies that mainly aimed at assessing the ELMOs transferability [2], especially by comparing it to the one of the widely used pseudoatoms [3]. Afterwards, an overview of the current possibilities offered by the recently constructed ELMO-libraries will be shown and, finally, future perspectives will be discussed in detail.

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