# Inclusion of electron correlation within the Interacting Quantum Atoms energy partition by means of closed shell coupled cluster theory

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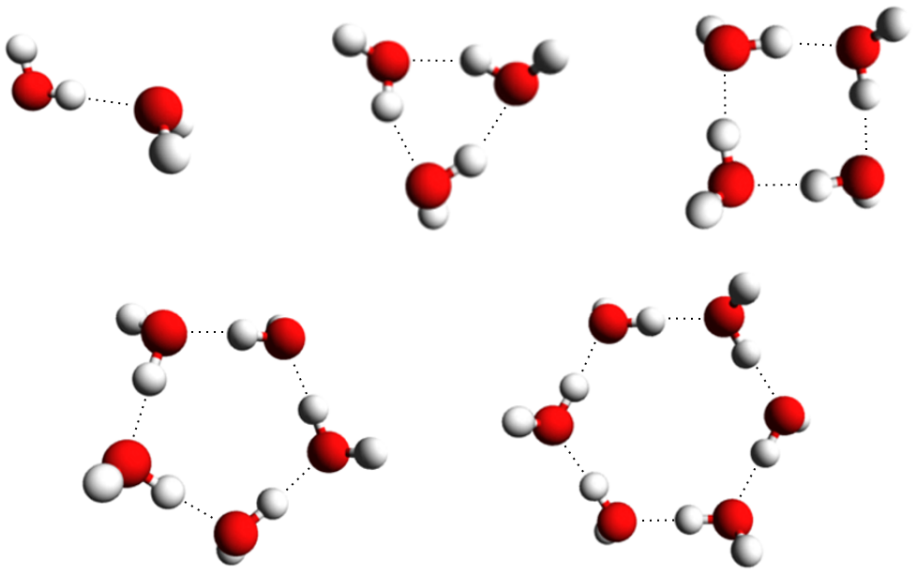
July 13, 2012

## Abstract

The interacting quantum atoms (IQA) is an energy decomposition of the energy of an electronic system which has found several applications[1] in virtue of its description of bonded, non-bonded and intermolecular interactions on the same footing. The IQA approach has been implemented for HF, full and truncated CI as well as CASSCF wavefunctions. Therefore, it is desirable to expand the IQA methodology so that it can be used along with methods which include electron correlation such as coupled cluster of Møller-Plesset perturbation theory. This seminar presents the construction of first and second-order density matrices in compliance with a closed shell coupled cluster energy. These density matrices provide the required input to carry out the energy partition in compliance with the IQA methodology. The present developments are discussed as potential tools for the study of non-covalent interactions.



[1]See for example: Martín Pendás Á., Francisco, E., Blanco M. A. and Gatti, C. *Chem. Eur. J.* **2007**, *13*, 9362–9371; Martín Pendás Á , Francisco E. and Blanco M. *Chem. Phys. Lett.* **2007**, *437*, 287–292; Martín Pendás Á, Francisco E., Blanco M. A. *J. Phys. Chem. A* **2006**, *110*, 12864–12869; García-evilla M., Francisco E., Costales, A., Martín Pendás, Á *J. Phys. Chem. A* **2012**, *116*, 1237–1250.