

Delocalisation measures on model metals at the correlated level

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Real space delocalisation indices (DIs) [1] have been set forth as measures of how deeply an electron network delocalises and the analysis of their decay trends with distance has been shown to allow us to characterise the metallic or insulating nature of real systems [2]. As these results are all based on uncorrelated Hartree-Fock (HF) calculations, we have lately put some effort on understanding the impact that the inclusion of Coulomb correlation has on simple model metallic systems, as exemplified by 1-dimensional hydrogen chains. We present here some of our results, paying particular attention to the relation existing between electron delocalisation, as measured by DIs, and the amount of electron correlation. We describe how the behavior of the indices is modified as Coulomb correlation is switched on progressively, going from non-correlated, HF descriptions towards complete active space (CAS) and full configuration interaction (FCI) levels.

[1] Bader, Richard FW. *Atoms in molecules*. John Wiley & Sons, Ltd, 1990.

[2] A. Gallo-Bueno, E. Francisco and A. Martín Pendás, in preparation.