Mössbauer spectroscopy for heavy elements: a 4-component relativistic study

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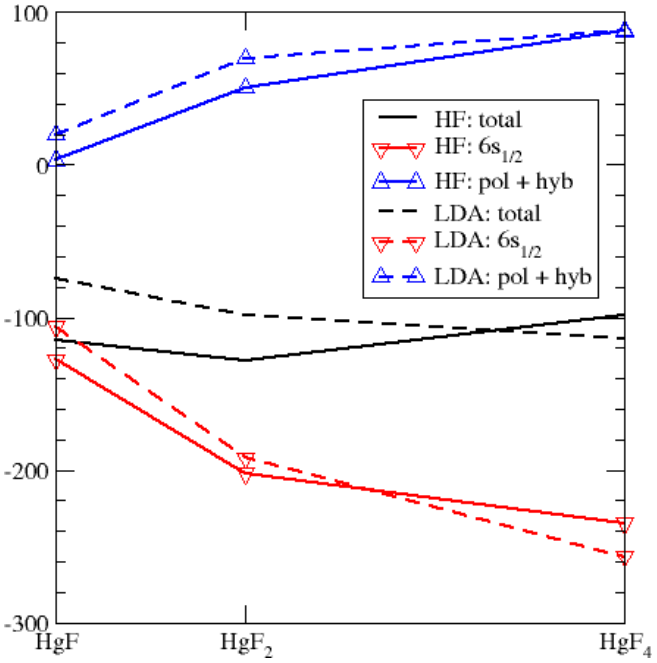

Figure 1: *Dominant contributions (in atomic units a_0^{-3}) to projection analysis of relative contact densities of mercury fluorides at the 4-component relativistic HF and LDA level.* pol=*polarization*, hyb=*hybridization*.

Mössbauer spectroscopy is an example of a spectroscopic technique showing extreme sensitivity to the electronic density in nuclear regions such that its modelling requires consideration of relativistic effects even for quite light species. In the present talk we report 4-component relativistic studies of the contact density (the density at the nucleus) of molecular species containing the Mössbauer active elements mercury[1] and xenon. We investigate the performance of relativistic density functional theory, using coupled-cluster calculations for calibration. We present a detailed analysis of the observed relative contact densities between molecular species, bringing into light the effect of polarization as well as overlap between ligands and the central atom. All calculations have been carried out with the DIRAC code for relativistic molecular calculations [2].

References

[1] Stefan Knecht, Samuel Fux, Robert van Meer, Lucas Visscher, Markus Reiher, and Trond Saue. Mössbauer spectroscopy for heavy elements: a relativistic benchmark study of mercury. *Theor. Chem. Acc.*, 2011. DOI: 10.1007/s00214-011-0911-2.

[2] DIRAC, a relativistic ab initio electronic structure program, Release DIRAC10 (2010), written by T. Saue, L. Visscher and H. J. Aa. Jensen, with contributions from R. Bast, K. G. Dyall, U. Ekström, E. Eliav, T. Enevoldsen, T. Fleig, A. S. P. Gomes, J. Henriksson, M. Iliaš, Ch. R. Jacob, S. Knecht, H. S. Nataraj, P. Norman, J. Olsen, M. Pernpointner, K. Ruud, B. Schimmelpfennig, J. Sikkema, A. Thorvaldsen, J. Thyssen, S. Villaume, and S. Yamamoto (see http://dirac.chem.vu.nl).