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Electronic structure of MX and MX_2 systems

(M = Cu, Ag, Au, X = F, Cl, Br)

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Potential energy functions of systems including a metal atom, and one or two halogen atoms (MX or MX_2), have been studied by ab−initio calculations.

In the present study, relativistic pseudo−potentials optimized in the group of H. Stoll (University of Stuttgart) were used. All molecular systems of interest were studied with similar linear space of configurations, considering only the highest two occupied electron shells. MRCI potential functions of the low−lying electronic singlet and triplet states, the dipole moment functions and the spectroscopic constants were calculated for the nine MX molecules. The results are compared with existing experimental data and previous theoretical calculations. The energy gap between the ground state and the excited states increases as the ionic character of the metal−halogen bond decreases, going from Cu to Au, whatever the halogen is.

Collinear cuts of the potential energy functions for MX_2 systems were obtained at the CCSD(T) or at the MRCI level of theory. Calculations of the three dimension potential energy functions and of the geometry dependence of the spin−orbit coupling for the lowest doublet states are in progress.