Theoretical study on electronic spectra and interaction in [Au 3]-L-[Au3] (L = C6F6,Ag+) complexes

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The electronic structure and spectroscopic properties of [Au 3(?-C(OEt) = NC6H4CH3) 3]n-(C6F6)m and [Au 3(?-C2,N3-bzim)3] n-(Ag+)m were studied at the B3LYP, PBE and TPSS levels. The interaction between the [Au3] cluster and L (C6F 6, Ag+) was analyzed. Grimme's dispersion correction is used for those functionals. Weak ?-interactions (Au-C6F 6) were found to be the main contribution short-range stability in the models; while in the models with Ag+, an ionic interaction is obtained. The absorption spectra of these models at the PBE level agree with the experimental spectra.