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Strengthening of Au-Au bonds in small gold clusters by adsorbing noble gases LUCA M. GHIRINGHELLI, SERGEY LEVCHENKO, MATTHIAS SCHEFFLER, Fritz-Haber-Institut, D-14195, Berlin — In state-of-the-art experiments for the vibrational spectra of metal clusters in the gas phase, photodissociation spectroscopy is performed on clusters complexed with noble gas (RG) atoms, where a RG atom is usually expected to form a weak van der Waals bond. By employing DFT (PBE functional with selected comparisons to PBE0, and to MP2 and CCSD(T) calculations), we surprisingly find a partially covalent bond of *neutral* dimers with RG. For RG = Ar, Kr, Xe one or two RG atoms can bind in a linear molecule with Au_2. While both Hirschfeld and Mulliken analyses show a small electron transfer from the RG to Au_2, the Au-Au bond *shortens* and the Au-Au stretch frequency increases. This is inconsistent with the expected effect of electron transfer to the antibonding orbital of the dimer. Electron-density (n) differences between the bonded systems and the isolated fragments show an accumulation of n between RG and the neighboring Au atom, and between the gold atoms. The analysis of the projected density of states reveals that, although only non-bonding orbital interactions and no charge transfer occurs between RG and Au_2, the d-electrons of Au_2 are redistributed due to the interaction with RG in such a way that the Au-Au σ_s bond is strengthened.

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