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Doping the golden buckyball: $M@Au_{16}^-$ clusters LEI-MING WANG, WEI HUANG, LAI-SHENG WANG, XIAOCHENG ZENG COLLABORATION, DETLEF SCHOOSS COLLABORATION — The 16-atom gold cluster (Au_{16}) was previously found to possess an unprecedentedly hollow cage structure. Using photoelectron spectroscopy and density functional theory, we have investigated the possibility of doping the Au_{16} cage with an external atom, $M@Au_{16}^-$ ($M = Cu, Ag, Zn, In, Si, Ge, Sn, Fe, Co, Ni$). We have found that doping the Au_{16}^- cluster with a Cu, Ag, Zn or In atom does not significantly alter its structure, and the dopant atom sits inside with little distortion to the parent cage. However, the Si, Ge, Sn, atoms cannot be doped inside the Au_{16} cage and they are found to completely change the structure of the parent cage due to the strong M-Au local interactions. The transition-metal-atom-doped species, $M@Au_{16}^-$ ($M = Fe, Co, Ni$), are found to be endohedral in nature with atomic-like magnetic moments and some minor structural distortions.

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