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Doping effects of sulfur and oxygen atoms on a golden cage

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The structural and electronic properties of XAu_{16}^- (X = S or O) have been studied by the scalar relativistic all-electron density functional calculations, in which a particular attention is paid to the stability of various XAu_{16}^- structures. We find that an X-encapsulated golden cage (XAu_{16}^-) represents an ionic character whereas in the other structures, adsorption characters are represented by covalent bonding. Especially, in $S@Au_{16}^-$, electrons are donated from the S atom to Au_{16}^-. The most stable XAu_{16}^- structures exhibit a small HOMO-LUMO energy gap, indicating that they could be chemically reactive. We also calculated the activation energy barriers of the transition between the most stable exohedral and endohedral adsorption configurations as well as their reaction energies. Our results demonstrate that the activation barrier in the OAu_{16}^- is lower than in SAu_{16}^-. This is associated with the smaller atomic radius of oxygen than that of sulfur.