

Au₁₁Re: A hollow or endohedral binary cluster?

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In this letter, we discussed the plausible formation of [Au₁₁Re] as a superatom with an electronic structure accounted by the 1S²1P⁶1D¹⁰ shell order, denoting similar stability to [W@Au₁₂]. The possible hollow or endohedral structures show a variable HOMO-LUMO gap according to the given structure (from 0.33 to 1.30 eV, at the PBE/ZORA level). Our results show that the energy minimum is an endohedral arrangement, where Re is encapsulated in a D_{3h}-Au₁₁ cage, retaining a higher gold-dopant stoichiometric ratio. This approach is useful for further rationalization and design of novel superatoms expanding the libraries of endohedral clusters. © 2018

Gold

Heteroatomic

Rhenium

Superatoms

Chemistry

Gold

Physical chemistry

Rhenium

Binary clusters

Endohedral clusters

Endohedral structure

Energy minima

Heteroatomic

HOMO-LUMO gaps

Stoichiometric ratio

Superatoms

