

Supplementary Information

The Ternary $C@Al_6Cu_4$ Cluster: Hexavalent Non-hybridized Carbon Atom and New Magic Number

Yassin A. Jeilani,^a Long Van Duong,^{b,c,*} Nguyen Minh Tam^d and Minh Tho Nguyen^{c,e}

^a Department of Chemistry, University of Hail, Hail, Saudi Arabia

^b Atomic Molecular and Optical Physics Research Group, Science and Technology Advanced Institute, Van Lang University, Ho Chi Minh City, Vietnam

^c Faculty of Applied Technology, School of Technology, Van Lang University, Ho Chi Minh City, Vietnam

^d Faculty of Basic Sciences, University of Phan Thiet, 225 Nguyen Thong, Phan Thiet City, Binh Thuan Province, Vietnam

^e Laboratory of Chemical Computation and Modeling, Institute for Computational Science and Artificial Intelligence, Van Lang University, Ho Chi Minh City, Vietnam

* Corresponding author: duongvanlong@vlu.edu.vn

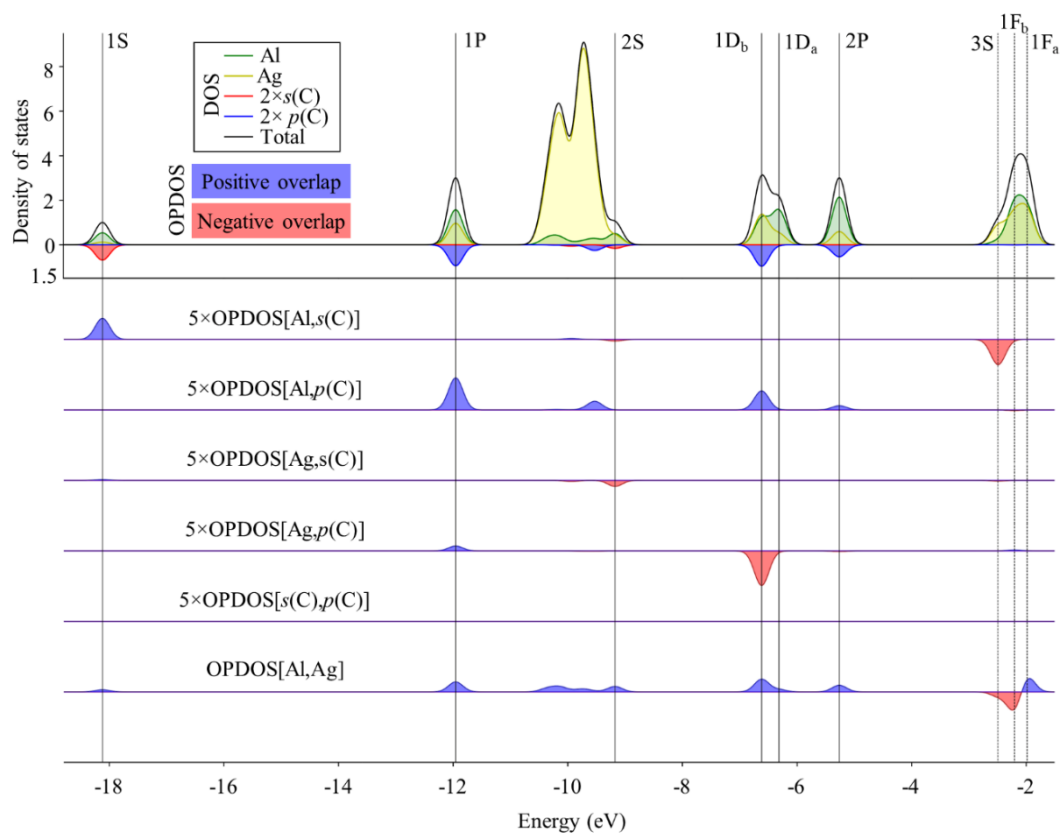


Figure S1. The partial and total densities-of-states (DOS) and the overlap population density-of-states (OPDOS) of $C@Al_6Ag_4$

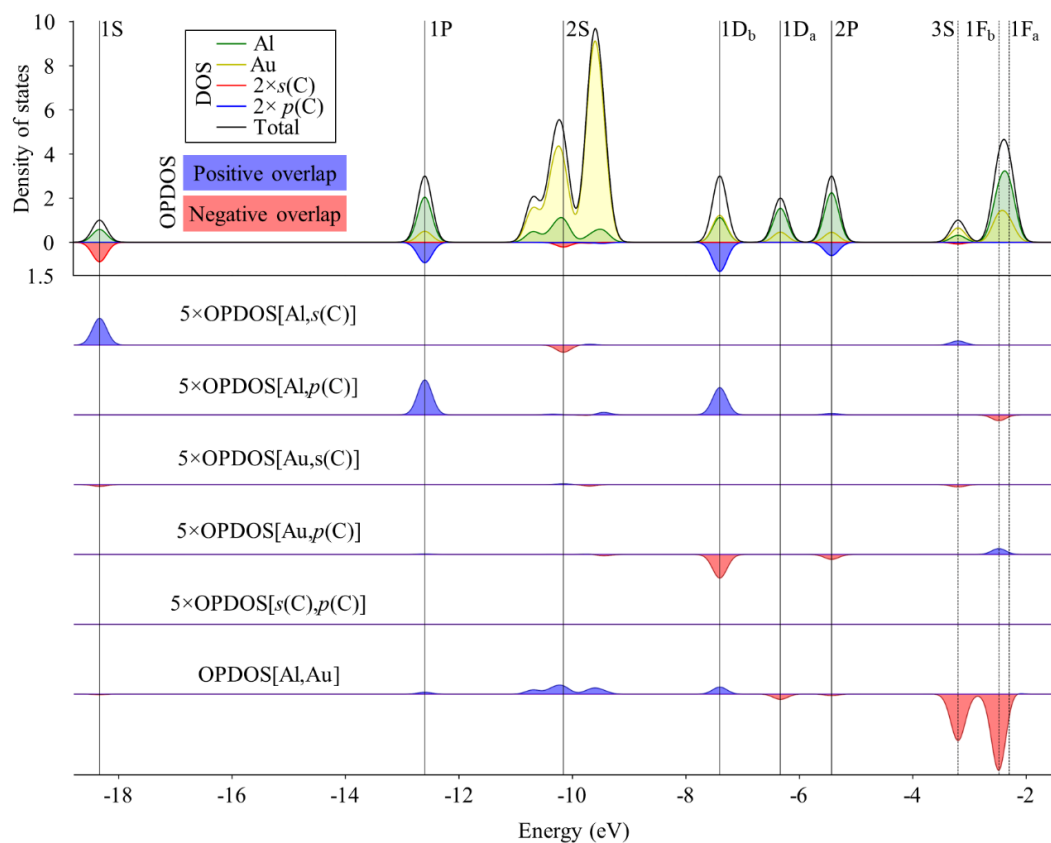


Figure S2. The partial and total densities-of-states (DOS) and the overlap population density-of-states (OPDOS) of $\text{C@Al}_6\text{Au}_4$.

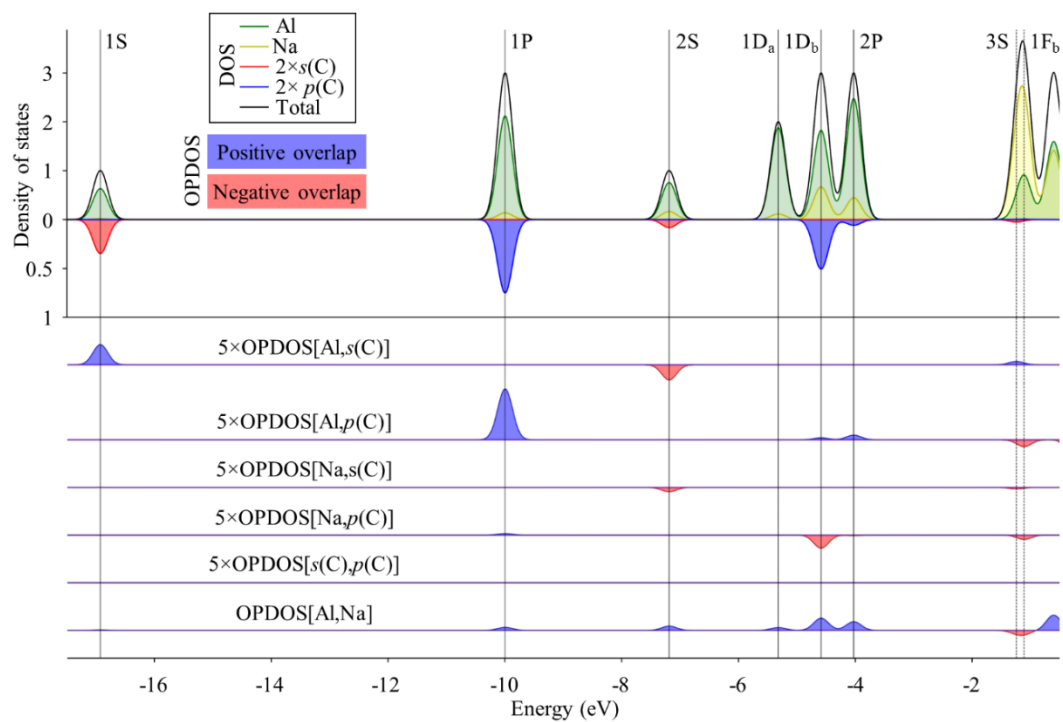


Figure S3. The partial and total densities-of-states (DOS) and the overlap population density-of-states (OPDOS) of $\text{C@Al}_6\text{Na}_4$.