Supporting Information for

From Isosuperatoms to Isosupermolecules: New Concepts in Cluster Science

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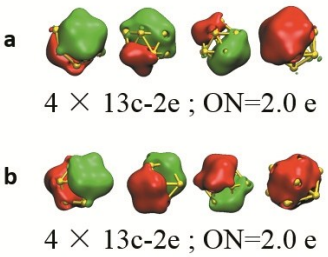

Figure S1: AdNDP localized natural bonding orbitals of two Au_{13}^{5+} clusters. (a) The Au_{13} with quasi-I_h symmetry*; (b) the Au_{13} with quasi-O_h symmetry.*

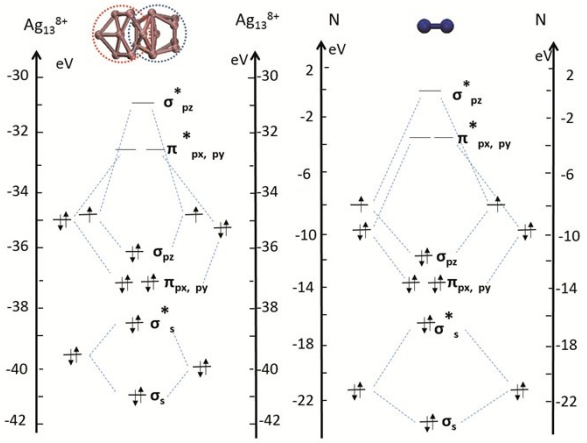

Figure S2. Schematic representation of the MO energy-level diagram for Ag_{22}^{12+}superatomic molecule (left, the energy calibration for two Ag_{13}^{8+} superatoms) and N_2 molecule (right, the energy calibration for N atoms).

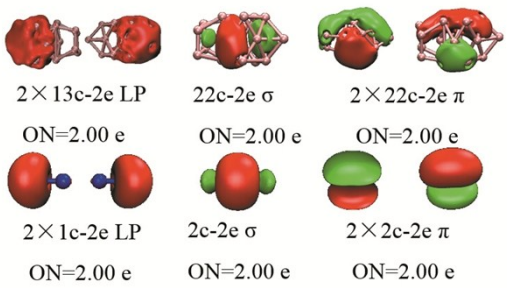

Figure S3: AdNDP localized natural bonding orbitals of Ag_{22}^{12+} and F_2.

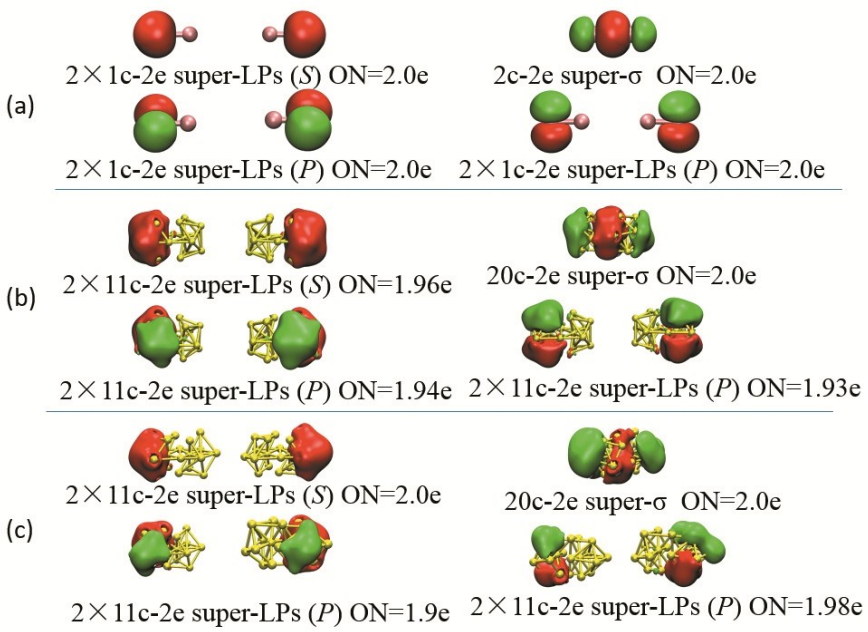

Figure S4:AdNDP localized natural bonding orbitals of F_2 and Au_{20}^{6+} cores. (a) F_2, (b) Au_{20}^{6+} core of $[Au_{20}(PPhpy_2)_{10}Cl_4]^{2+}$, (c) Au_{20}^{6+} core of $Au_{30}S(StBu)_{18}$.