

# **Survey of Short and Long Cuprophilic $d^{10}$ - $d^{10}$ Contacts for Tetranuclear Copper Clusters. Understanding of Bonding and Ligand Role from A Planar Superatom Perspective**

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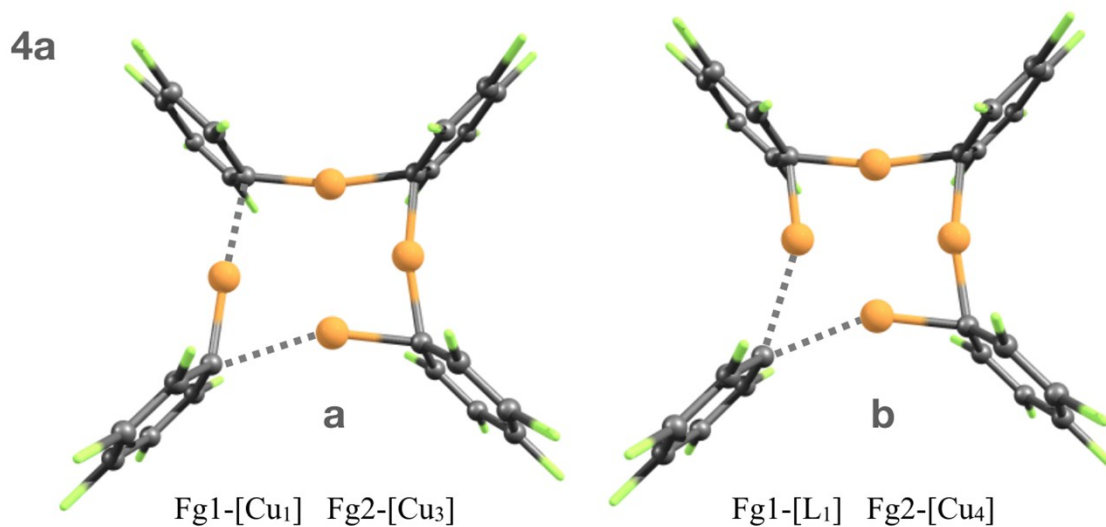
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## **Supplementary Information**

**Table S1.** The energy of decomposition analysis (EDA kcal.mol<sup>-1</sup>) for the selected interacting fragments [Au<sub>4</sub>]<sup>4+</sup>-[L<sub>4</sub>]<sup>4-</sup>.

| EDA (kcal/mol) <sup>1</sup>                                            | 1b       | 2b       | 3b       | 4b       | 5b       |
|------------------------------------------------------------------------|----------|----------|----------|----------|----------|
| Frag. [Au <sub>4</sub> ] <sup>4+</sup> [L <sub>4</sub> ] <sup>4-</sup> |          |          |          |          |          |
| ΔE <sub>Pauli</sub>                                                    | 1121.63  | 1159.25  | 1026.20  | 1001.32  | 1102.82  |
| ΔE <sub>elstat</sub>                                                   | -1958.87 | -1898.93 | -1930.58 | -1806.84 | -964.98  |
| ΔE <sub>orb</sub>                                                      | -1145.78 | -1241.13 | -1061.25 | -1021.19 | -885.69  |
|                                                                        |          |          |          |          |          |
| ΔE <sub>Disp</sub>                                                     | -22.70   | -23.05   | -31.50   | -15.00   | -20.91   |
| ΔE <sub>Def</sub>                                                      | 24.48    | 8.24     | 8.12     | 19.28    | 7.40     |
| ΔE <sub>int</sub>                                                      | -2005.69 | -2003.85 | -1997.14 | -1841.07 | -1850.68 |
|                                                                        |          |          |          |          |          |
| <i>Superatomic Levels</i>                                              |          |          |          |          |          |
| 1S                                                                     | 1.22     | 1.90     | 0.87     | 1.81     | 0.64     |
| 1P <sub>x</sub>                                                        | 0.55     | 0.64     | 0.47     | 0.57     | 0.63     |
| 1P <sub>y</sub>                                                        | 0.54     | 0.65     | 0.50     | 0.59     | 0.59     |
| 1D <sub>xy</sub>                                                       | 0.35     | 0.38     | 0.31     | 0.27     | 0.46     |



**Figure S1.** The corresponding fragmentation that involve the obtaining of a clean dispersion energy.