

**Table S1**  $\beta_0$  values of CuAg@Ca<sub>7</sub>Be(1) at MP2 method in conjunction with the different basis set for Be/Mg/Ca and lan12dz basis set for Cu and Ag.

| CuAg@Ca <sub>7</sub> Be(1) | $\beta_0$ (au) |
|----------------------------|----------------|
| 6-31+g                     | 8600           |
| 6-31+g(d)                  | 8600           |
| 6-311+g                    | 8900           |
| 6-311+g(d)                 | 9700           |
| 6-311+g(2d)                | 12000          |
| 6-311+g(3d)                | 12000          |
| 6-311+g(3df)               | 12000          |

**Table S2**  $\beta_0$  values of five electroneutral molecules at MP2 method in conjunction with the different basis set for Be/Mg/Ca and lan12dz basis set for Cu and Ag.

| $\beta_0$ (au)             | 6-311+g(2d) | 6-311+g(3d) | 6-311+g(3df) |
|----------------------------|-------------|-------------|--------------|
| CuAg@Ca <sub>8</sub>       | 5800        | 6500        | 6500         |
| CuAg@Ca <sub>7</sub> Mg(3) | 7300        | 7400        | 7300         |
| CuAg@Ca <sub>7</sub> Be(3) | 9400        | 9300        | 9300         |
| CuAg@Ca <sub>7</sub> Be(1) | 12000       | 12000       | 12000        |
| CuAg@Ca <sub>7</sub> Mg(1) | 13500       | 14300       | 14300        |

**Table S3** The Associated Energies for an Atom with Label  $n$ ,  $E_b$ (kcal/mol)

| n                         | 1     | 2     | 3     | 4     | 5     | 6     | 7     | 8     |
|---------------------------|-------|-------|-------|-------|-------|-------|-------|-------|
| CuAg@Ca <sub>8</sub>      |       |       | 38.09 |       |       |       |       | 29.92 |
| CuAg@Ca <sub>7</sub> Mg-3 | 30.51 | 29.68 | 33.69 | 36.39 | 42.06 | 36.39 | 29.68 | 30.51 |
| CuAg@Ca <sub>7</sub> Be-3 | 37.70 | 36.70 | 59.07 | 37.35 | 34.82 | 33.93 | 32.60 | 38.17 |
| CuAg@Ca <sub>7</sub> Be-1 | 52.30 | 26.86 | 41.43 | 36.60 | 35.39 | 36.42 | 41.53 | 38.17 |
| CuAg@Ca <sub>7</sub> Mg-1 | 26.43 | 32.73 | 39.04 | 37.18 | 37.18 | 39.04 | 31.13 | 31.13 |