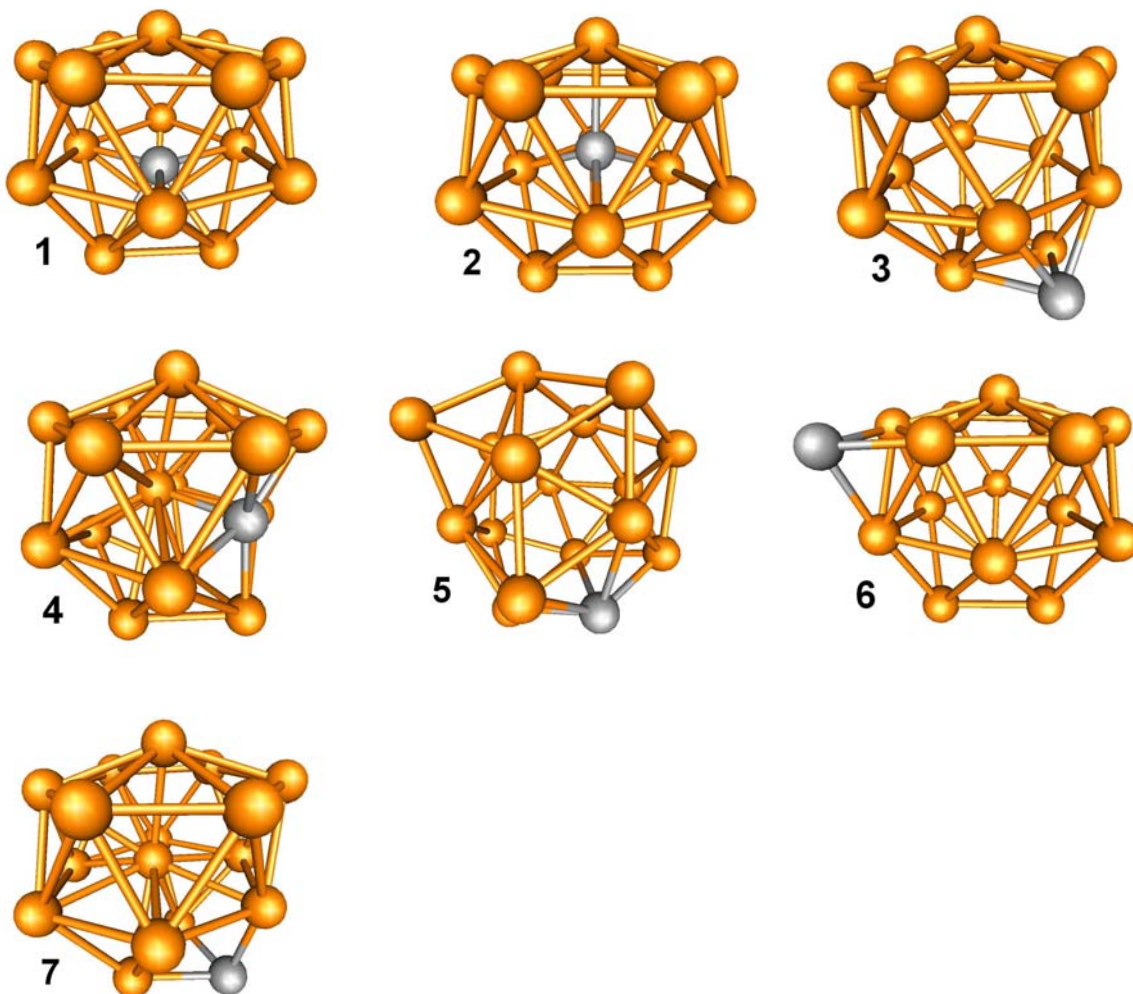


## SUPPORTING INFORMATION

*Michael Walter and Hannu Häkkinen: A hollow tetrahedral cage of hexadecagold dianion provides a robust backbone for a tunable sub-nanometer oxidation and reduction agent via endohedral doping*

**Local minima for Si@Au<sub>16</sub> and Al@Au<sub>16</sub>.** The images show geometries found for Si@Au<sub>16</sub>. Al@Au<sub>16</sub> has corresponding geometries but with slightly different bond lengths. The coordinates of these structures are available at: <http://nano.jyu.fi/groups/comps/GoldMine>. The table shows the relative energies (in eV) of the structures with respect to the off-center-doped ground state **1**.



	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>	<b>5</b>	<b>6</b>	<b>7</b>
Si@Au <sub>16</sub>	0	0.16	0.40	0.77	0.78	0.79	1.30
Al@Au <sub>16</sub>	0	0.03	0.66	1.03	0.50	1.21	1.02