Supporting Information

The Encapsulated Lithium Effect of Li@C_{60}Cl_{8} Remarkably Enhances the Static First Hyperpolarizability

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Table S1. The NBO charge of all the atoms in C_{60} (C_{2v}), C_{60}Cl_{8} and Li@C_{60}Cl_{8} at B3LYP/6-31G(d) level

<table>
<thead>
<tr>
<th>Atom</th>
<th>Li@C_{60}Cl_{8}</th>
<th>C_{60}Cl_{8}</th>
<th>C_{60} (C_{2v})</th>
<th>Li@C_{60}C_{8}</th>
<th>C_{60}C_{8}</th>
<th>C_{60} (C_{2v})</th>
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