Electronic Supplementary Information

Graphyne-Anchored Single Fe Atoms as Efficient CO Oxidation Catalyst as Predicted by DFT Calculations

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2. Calculated deformation electron densities of Fe atom adsorbed on pristine (left) and SAV-αGy.
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<th>B12</th>
<th>T1</th>
<th>T2</th>
<th>B11</th>
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<td>-2.91</td>
<td>-0.45</td>
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**Figure S1.** Optimized structures and binding energies of all studied single Fe atom adsorbed on pristine 2D αGy.
**Figure S2** Calculated deformation electron densities of Fe atom adsorbed on pristine (left) and SAV-αGy.