Electronic Supplementary Information

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

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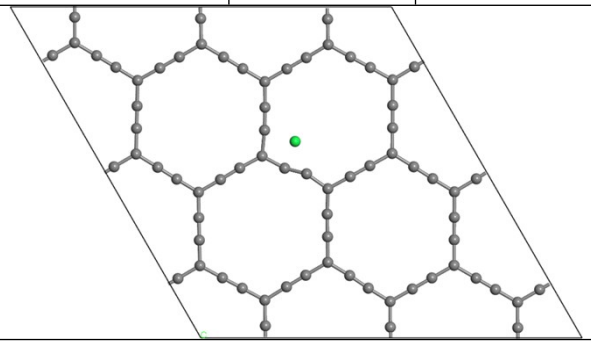
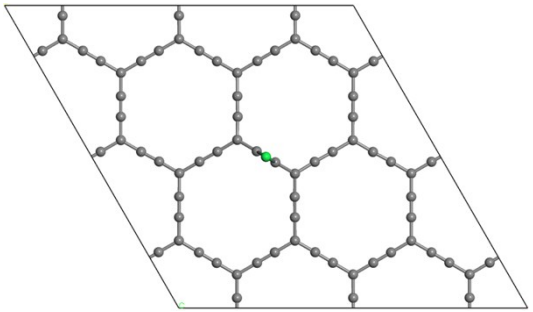
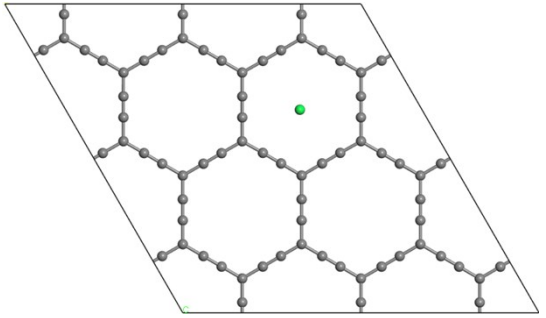
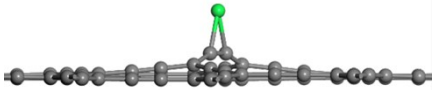
Top View					
Side View					
E_b (eV)	-3.36			-2.91	-0.45

Figure S1. Optimized structures and binding energies of all studied single Fe atom adsorbed on pristine 2D αGy.

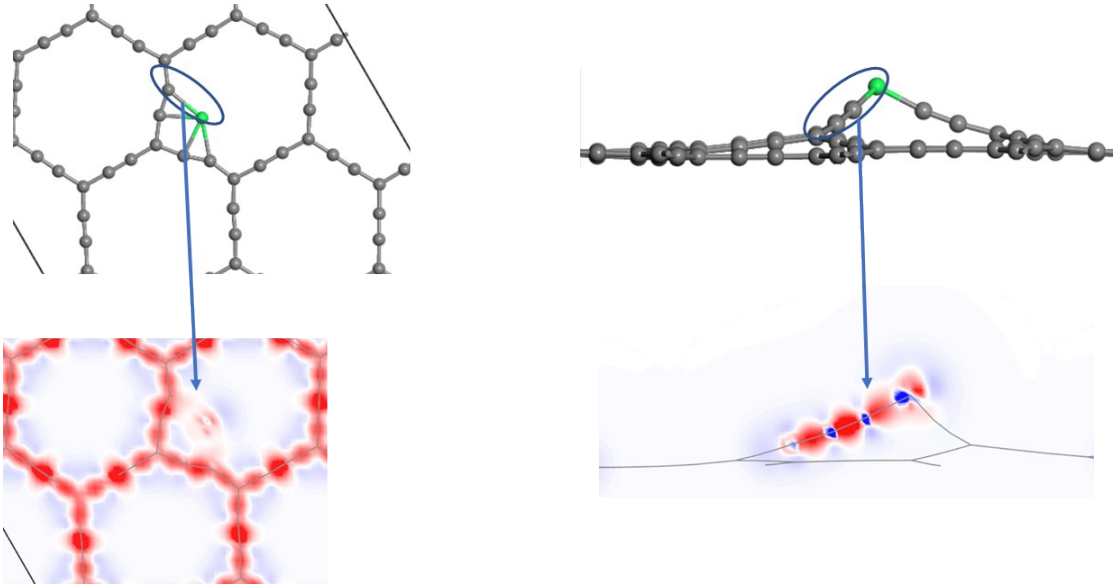


Figure S2 Calculated deformation electron densities of Fe atom adsorbed on pristine (left) and SAV-αGy.