Supplementary Materials for: Hydrogen-designed spin-states of 2D silicon carbide and graphene nanostructures

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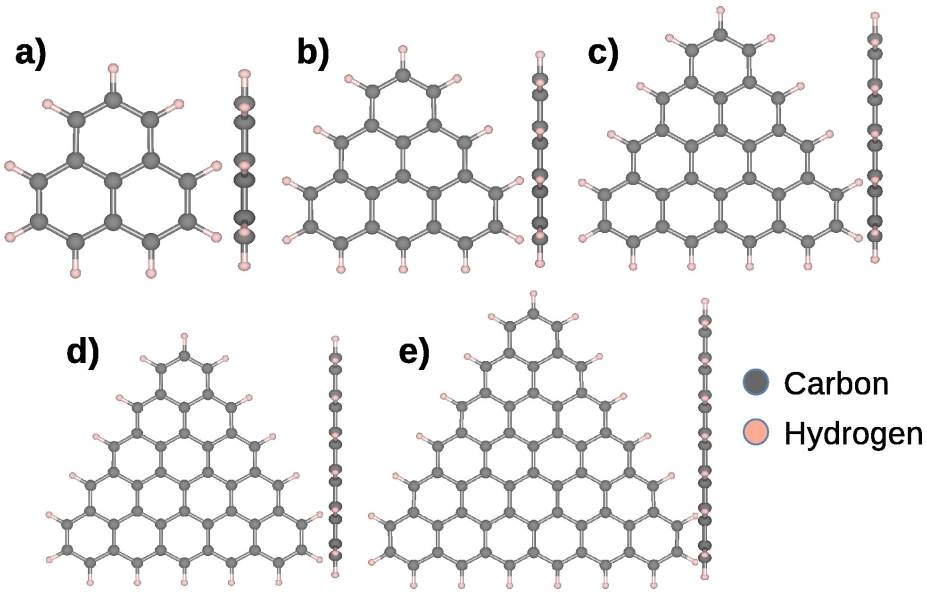

Figure 1: Top and side views of ground state geometries obtained at B3LYP/def2-SVP level of theory for N_R-GRt with $N_R = 2 - 6$.

Table 1: Formation energy for the adsorbed hydrogen atoms on both N_R-SiC and N_R-GRt systems, calculated for all three sublattice adsorption cases A, B, and AB.

system	sublattice	adsorbed energy (eV)
3-GRt	sub-a	-1.59
	sub-ab	-1.57
	sub-b	-0.82
6-GRt	sub-a	-1.33
	sub-ab	-1.49
	sub-b	-0.88
3-SiCt	sub-a	-2.88
	sub-ab	-2.42
	sub-b	-1.60
6-SiCt	sub-a	-2.65
	sub-ab	-2.36
	sub-b	-1.38

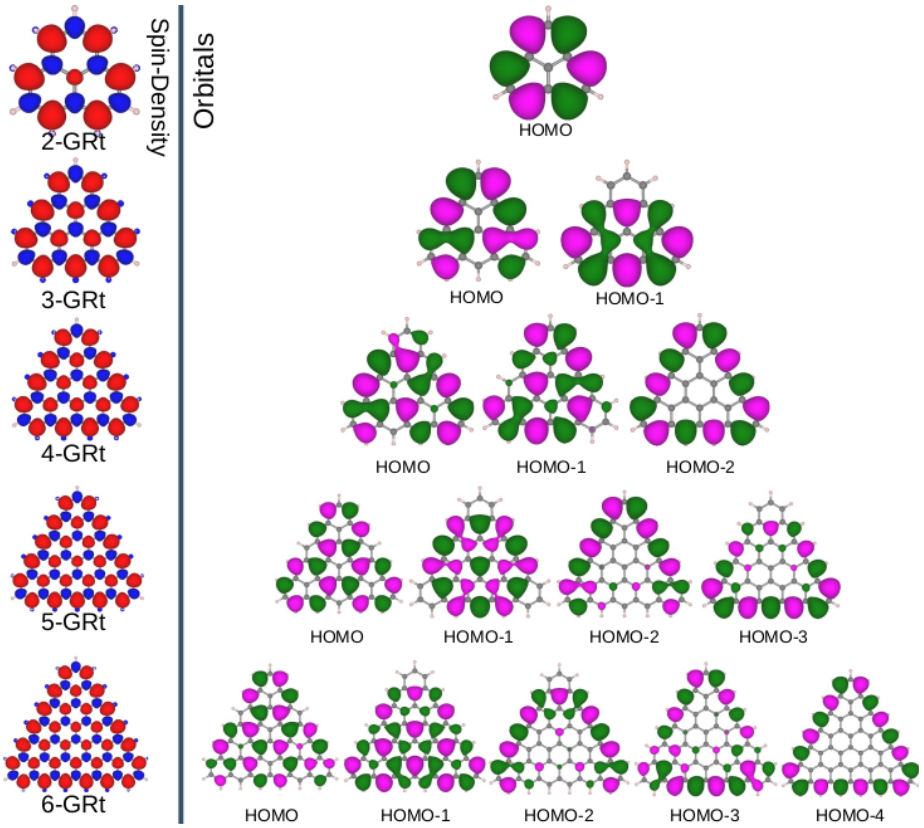

Figure 2: Spin density and open shell molecular orbitals for N_R-GRt systems. iso-surface = 0.002, and =0.015 for the spin density and molecular orbitals respectively.

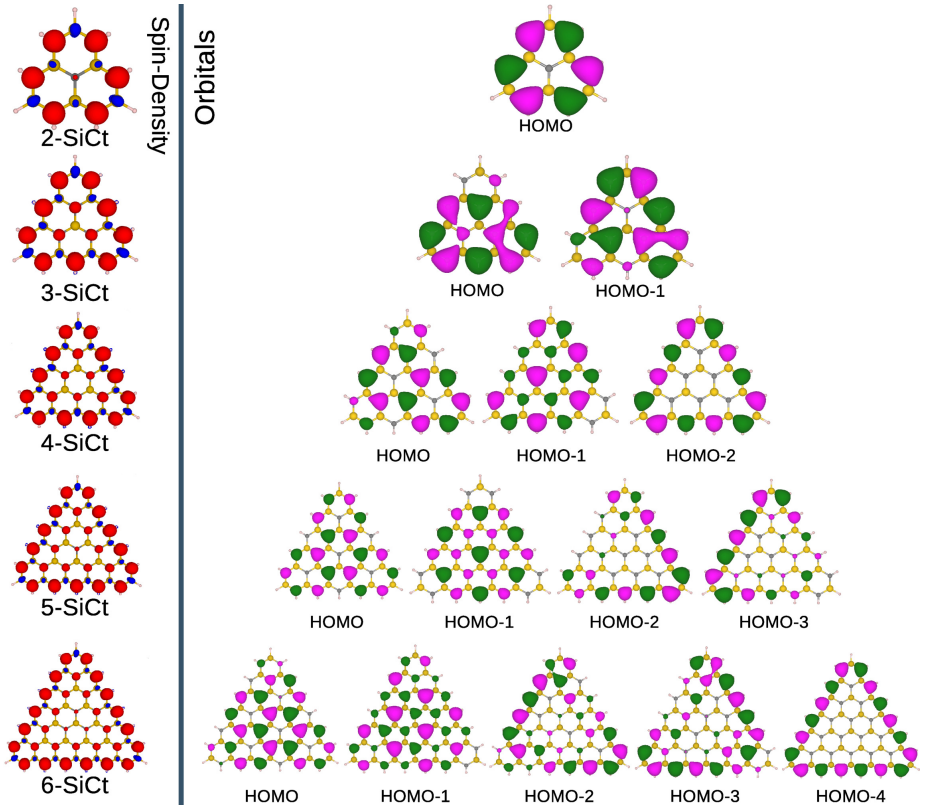

Figure 3: Spin density and open shell molecular orbitals for N_R-SiCt systems, iso-surface = 0.002, and =0.015 for the spin density and molecular orbitals respectively

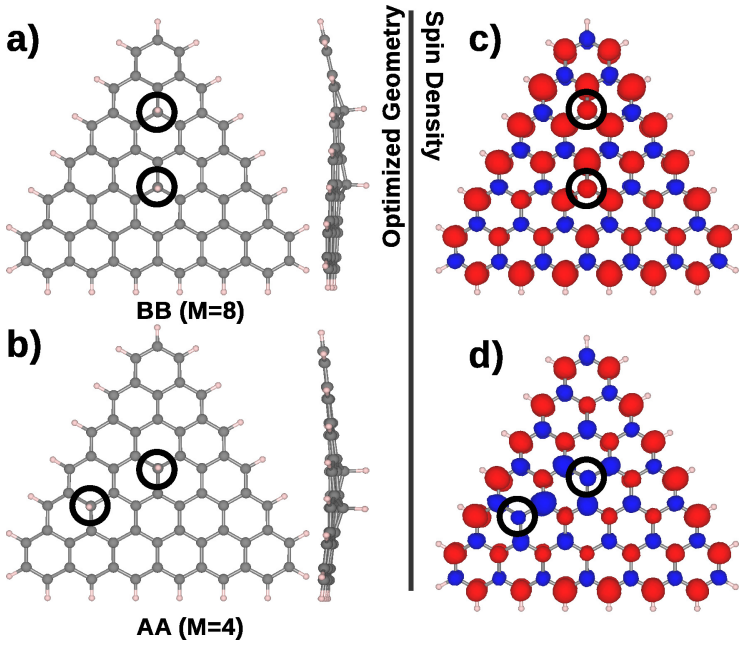

Figure 4: Spin density and open shell molecular orbitals for N_R-SiCt systems, iso-surface = 0.002, and =0.015 for the spin density and molecular orbitals respectively

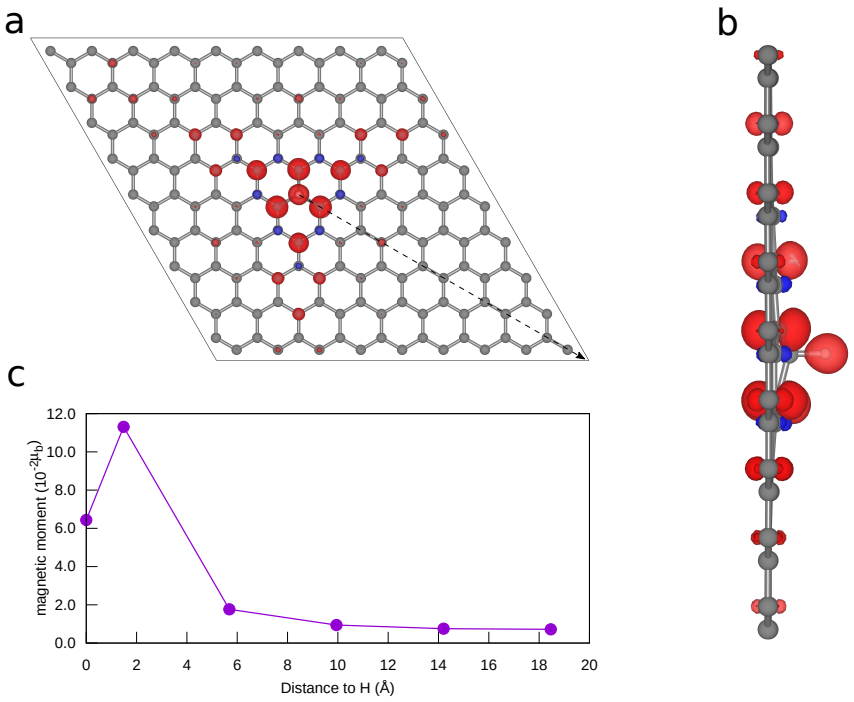

Figure 5: Figure (a) depicts the spin density of a hydrogen atom adsorbed in a 9x9 GR supercell from both the top and (b) side views. The isosurface set was 0.002. The red (blue) region represents positive (negative) spin density values, while the dotted arrow indicates the path taken to create the magnetic moment vs. distance graph. (c) Display the variation in the magnetic moment in relation to the site's in-plane distance from the H. The dots on the graph represent the opposite sub-lattice where H was adsorbed; the same sub-lattice values were not plotted because the magnetic moment was small and practically constant.