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Supporting Information for

Surface Modification of Graphene with Functionalized Carbenes and Their Applications in The Sensing of Toxic Gases: A DFT Study.

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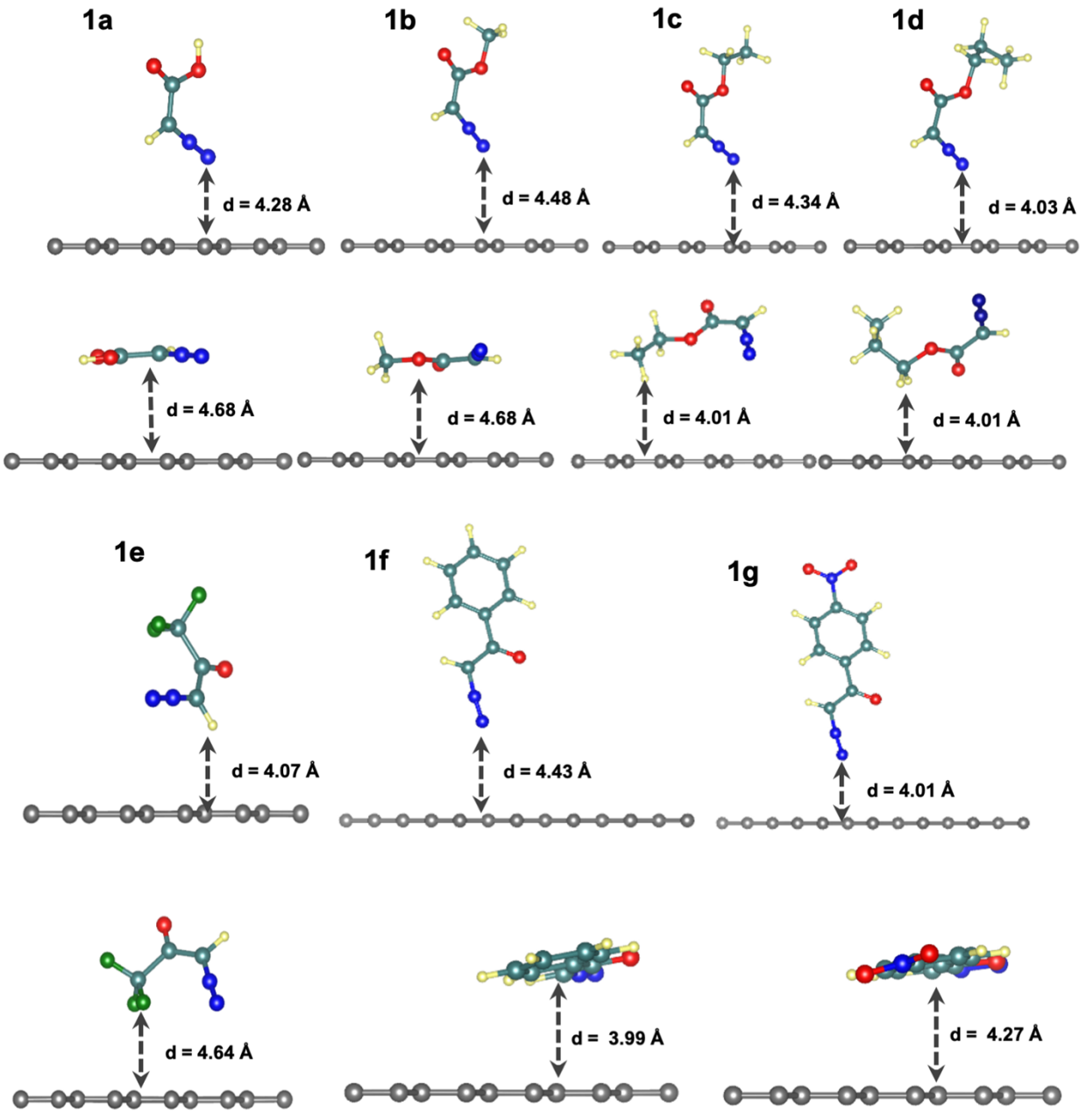

Figure S1. Relaxed geometries of horizontally and vertically physiosorbed diazomethane **1(a-g)** on 5×5 graphene supercell. Values are for the distances between the closest atom to graphene and the graphene surface depicted from lateral and top views.

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Table S1. The geometrical parameters and reaction energies of cyclopropane-modified graphene derivatives on 5´5 graphene supercells

Adsorbates	E_{ads}(eV)	d^1 (Å)	d^2(Å)	d^3(Å)	d^4(Å)	d^5(Å)	α(°)	β(°)	h(Å)
3a	-1.67	1.56	1.56	1.54	1.22	0.98	60.3°	117.6°	0.6
3b	-1.65	1.54	1.55	1.55	1.22	1.35	60.3°	117.5°	0.6
3c	-1.60	1.52	1.52	1.57	1.22	1.35	62.3°	117.3°	0.7
3d	-1.64	1.54	1.52	1.56	1.22	1.36	61.1°	117.2°	0.7
3e	-1.71	1.59	1.57	1.52	1.22	1.56	57.7	117.9°	0.6
3f	-1.33	1.57	1.56	1.54	1.21	1.50	58.8°	117.9°	0.6
3g	-1.39	1.58	1.56	1.53	1.24	1.51	58.1°	118.0°	0.6