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First-principles study of SiC and GeC monolayers adsorb ed with non-metal atoms

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Table S1: Adsorption energy E_{ad} (eV), band gap (eV), and total magnetic moment M_t (μ_B) in SiC and GeC monolayers adsorbed with H, O, and F atoms using vacuum width of 14/20 Å.

		E_{ad}	**Band gap**		**M_t**
			Spin-up	Spin-down	
SiC					
	H	-0.60/-0.59	2.58/2.58	0.03/0.04	1/1
	O	-0.89/-0.88	1.88/1.87	1.88/1.87	0/0
	F	-3.02/-3.01	M/M	M/M	0/0
GeC					
	H	-0.95/-0.94	0.45/0.44	1.66/1.65	1/1
	O	-0.63/-0.62	1.68/1.68	1.68/1.68	0/0
	F	-3.49/-3.48	2.18/2.18	0.06/0.06	1/1

Table S2: Adsorption energy E_{ad} (eV), band gap (eV), and total magnetic moment M_t (μ_B) in SiC and GeC monolayers adsorbed with H, O, and F atoms calculated with DFT-D3/DFT-D2 method.

		E_{ad}	**Band gap**		**M_t**
			Spin-up	Spin-down	
SiC					
	H	-0.60/-1.71	2.58/2.58	0.03/0.03	1/1
	O	-0.89/-2.00	1.88/1.87	1.88/1.87	0/0
	F	-3.02/-4.14	M/M	M/M	0/0
GeC					
	H	-0.95/-2.87	0.45/0.45	1.66/1.66	1/1

	O	-0.63/-2.55	1.68/1.68	1.68/1.68	0/0
	F	-3.49/-5.42	2.18/2.18	0.06/0.06	1/1

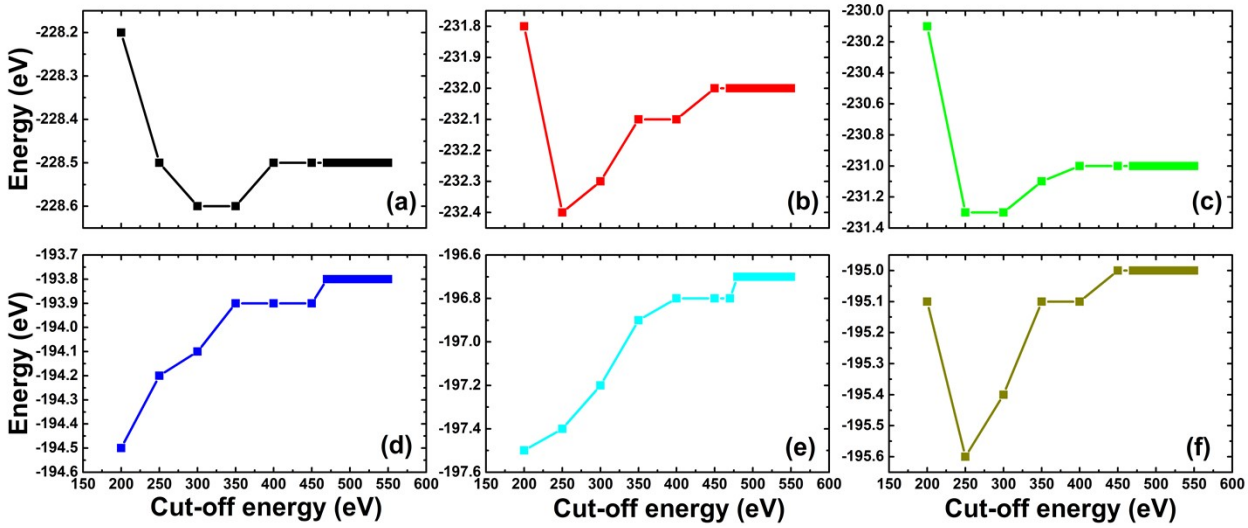

Figure S1: Energy of SiC monolayer adsorbed with (a) H, (b) O, and (c) F; and GeC monolayer adsorbed with (d) H, (e) O, and (F) calculated with different cut-off energies.

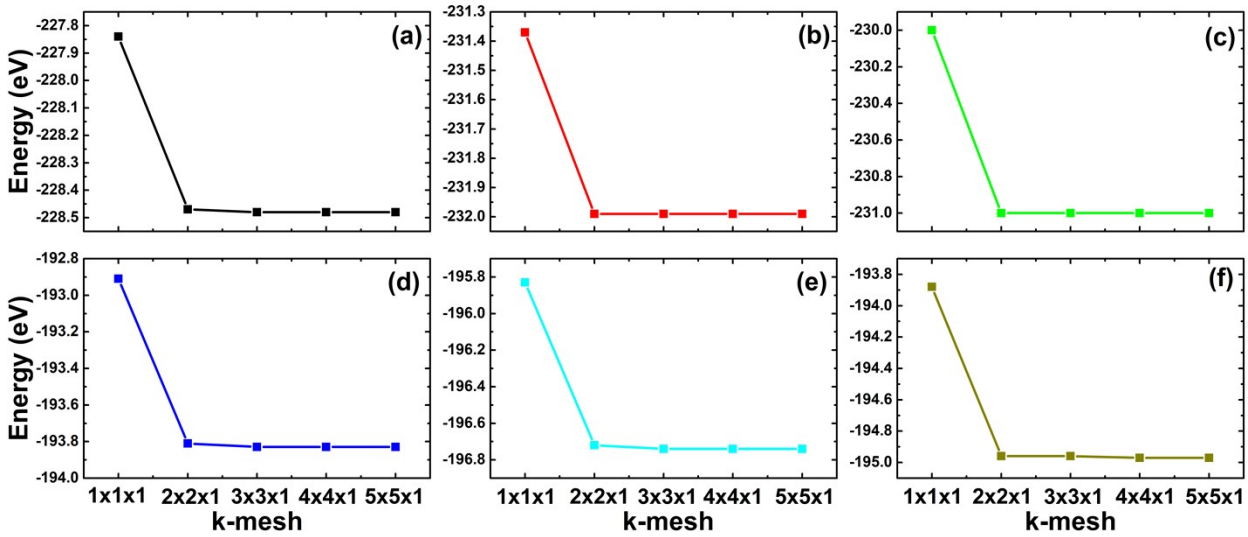

Figure S2: Energy of SiC monolayer adsorbed with (a) H, (b) O, and (c) F; and GeC monolayer adsorbed with (d) H, (e) O, and (F) calculated with different k-meshes.

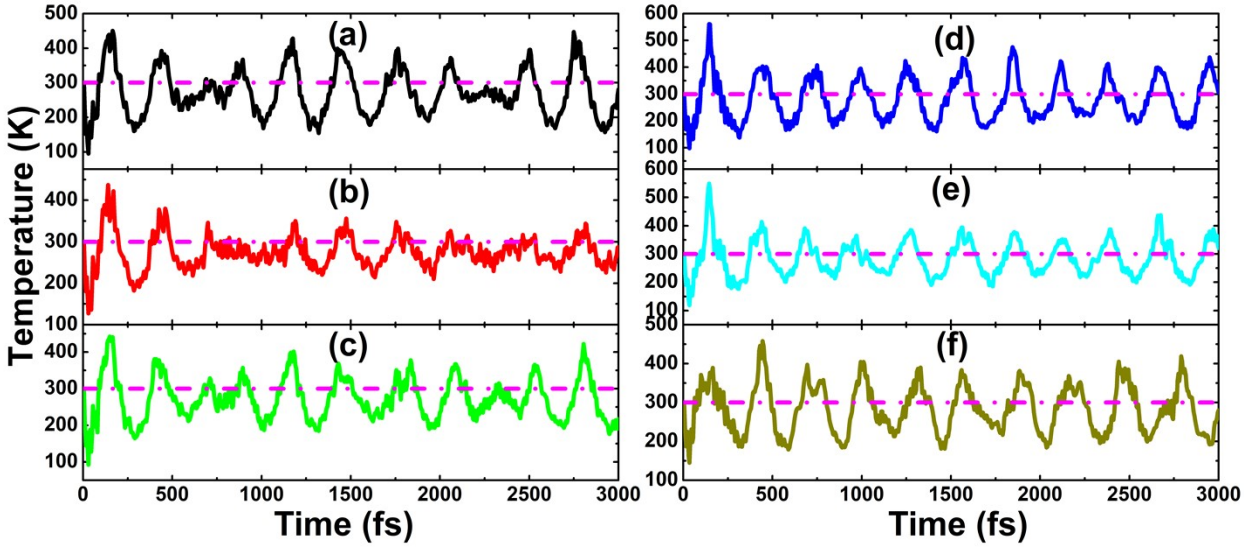

Figure S3: AIMD simulations at 300 K of SiC monolayer adsorbed with (a) H, (b) O, and (c) F; and GeC monolayer adsorbed with (d) H, (e) O, and (F).