

Novel Electronic and Magnetic Features in XC (X = Si and Ge) Monolayers Induced by Doping With VA-group Atoms

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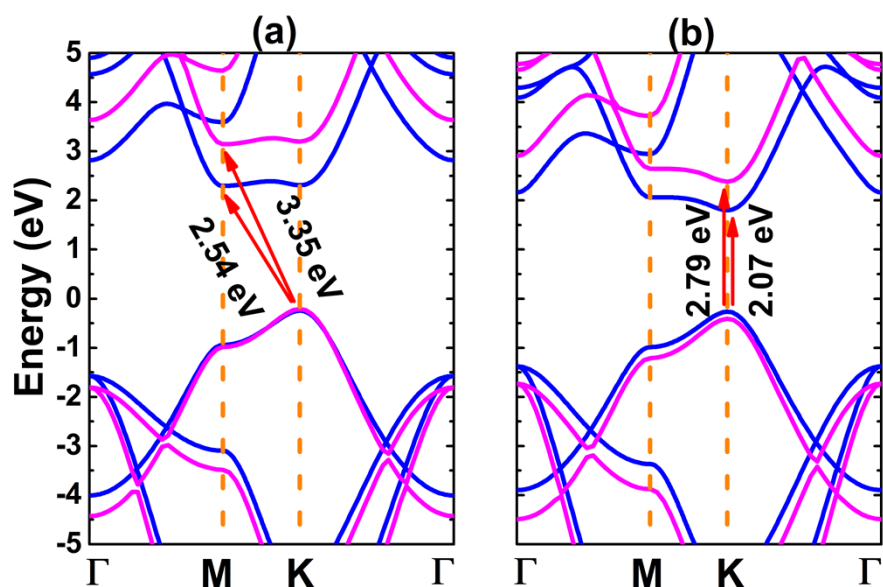


Figure S1: Electronic band structure (Blue curve: PBE; Pink curve: HSE06; The Fermi level is set to 0 eV) of (a) SiC and (b) GeC monolayer.

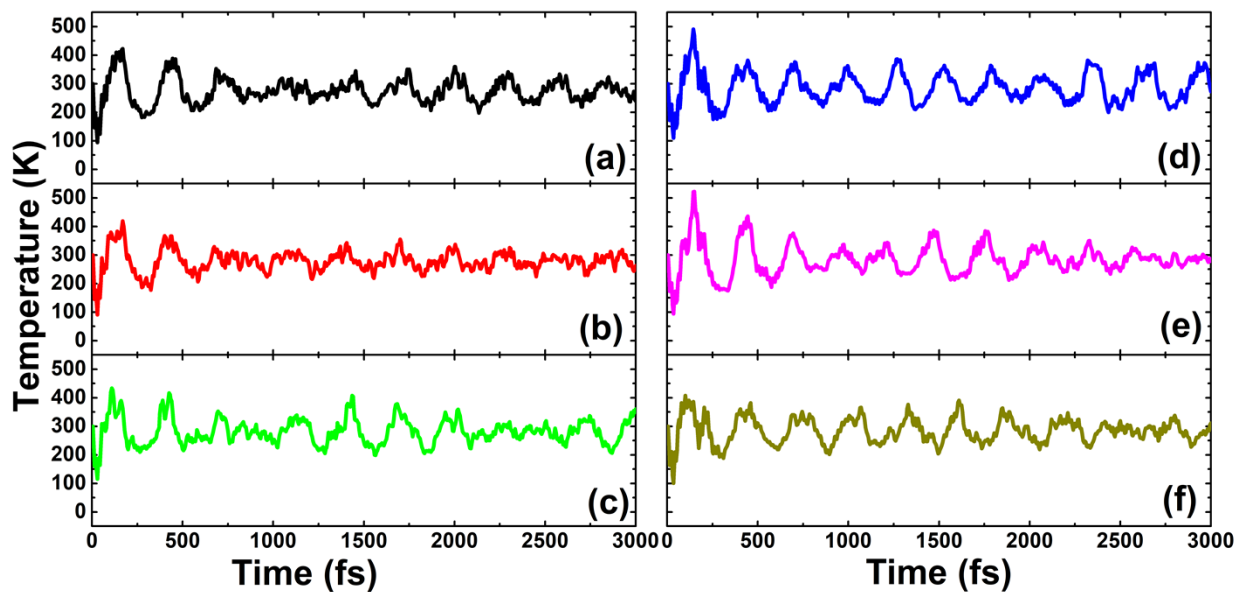


Figure S2: AIMD simulations of (a) N-, P-, and As-doped SiC monolayer; (d) N-, (e) P-, and (f) As-doped GeC monolayer at 300 K.

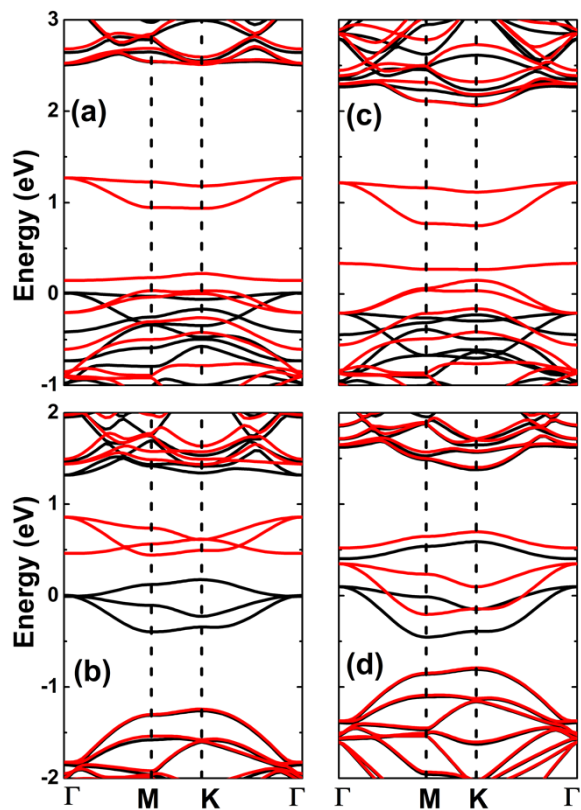


Figure S3: Electronic band structure (Spin-up: Black curve; Spin-down: Red curve; The Fermi level is set to 0 eV) of SiC monolayer with (a) Si single vacancy and (b) C vacancy, and of GeC monolayer with (c) Ge single vacancy and (d) C single vacancy.

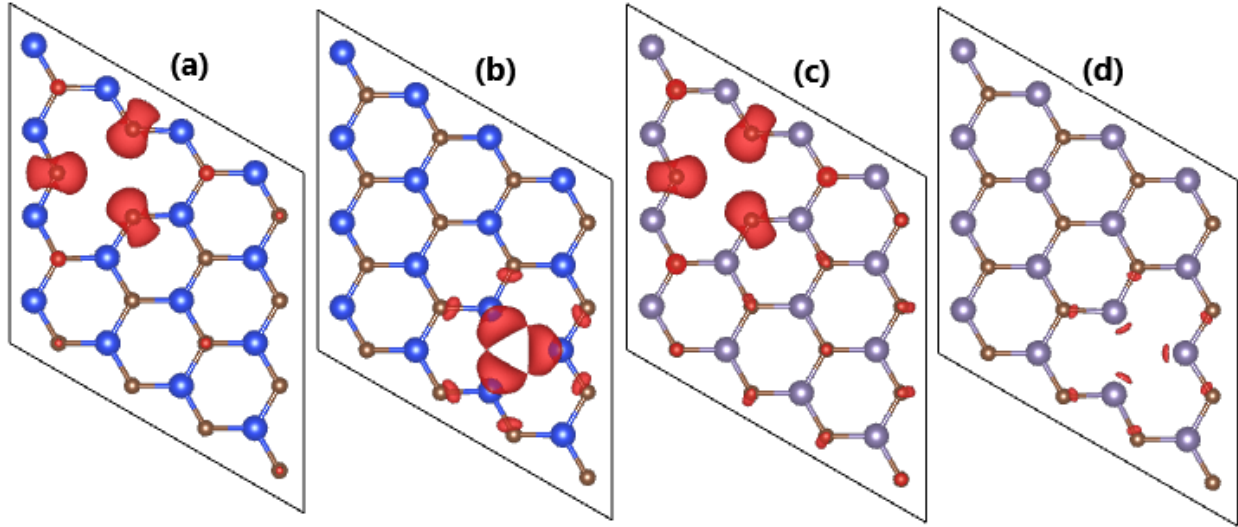


Figure S4: Spin density (Iso-surface value: 0.008; Red surface: Spin-up; Green surface: Spin-down) in SiC monolayer with (a) Si single vacancy and (b) C vacancy, and of GeC monolayer with (c) Ge single vacancy and (d) C single vacancy.

Table S1: Electronic band gap E_g (spin-up/spin-down; M = metal), Electronic character (M = metal; HM = half-metallic), and total magnetic moment M_t of SiC and GeC monolayers with single vacancies.

	SiC monolayer		GeC monolayer	
	Si single vacancy	C single vacancy	Ge single vacancy	C vacancy
E_g (eV)	M/M	M/1.69	2.27/M	M/M
Electronic character	M	HM	HM	M
M_t (μ_B)	3.19	2.00	4.00	0.87