Supplementary Material

High elastic moduli, controllable bandgap and extraordinary carrier mobility in single-layer diamond

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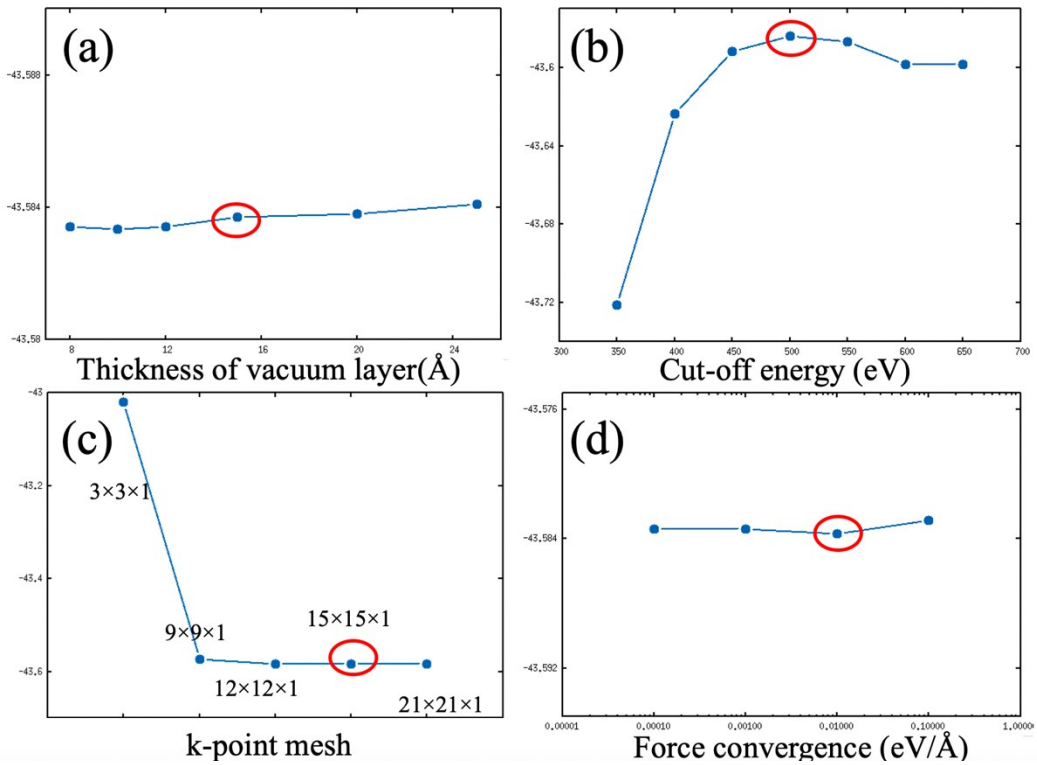

Figure S-1. The total energies of FD with respect to the (a) thickness of vacuum layer, (b) cut-off energy, (c) k-point mesh, and (d) force convergence. The red circles denote the used parameters in the present study.

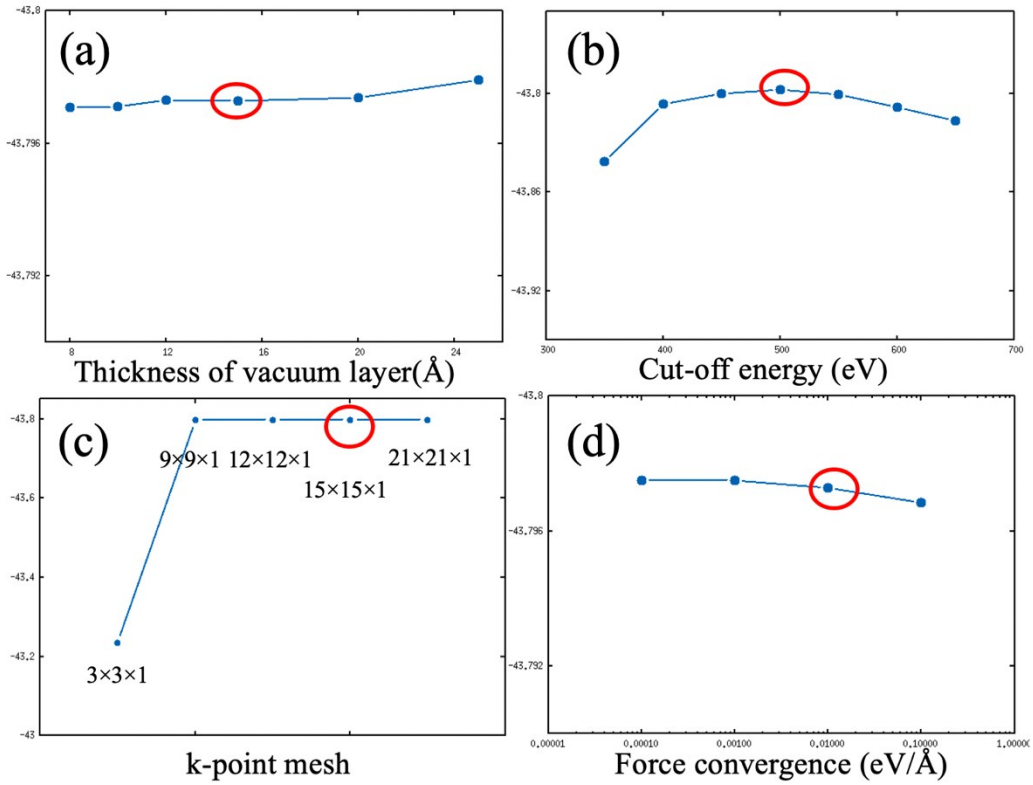

Figure S-2. The total energies of HD with respect to the (a) thickness of vacuum layer, (b) cut-off energy, (c) k-point mesh, and (d) force convergence. The red circles denote the used parameters in the present study.

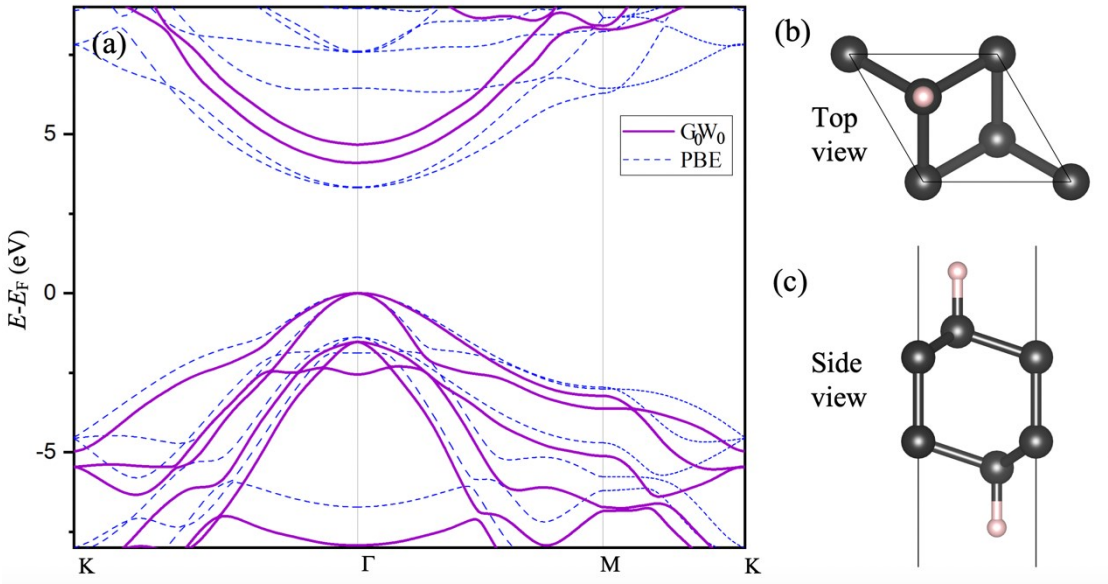

Figure S-3. (a) Band structure of HD by using the PBE (dotted) and G_0W_0 (solid) methods. (b, c) Top (b) and side views (c) of HD with carbon (hydrogen) atoms colored in black (white).

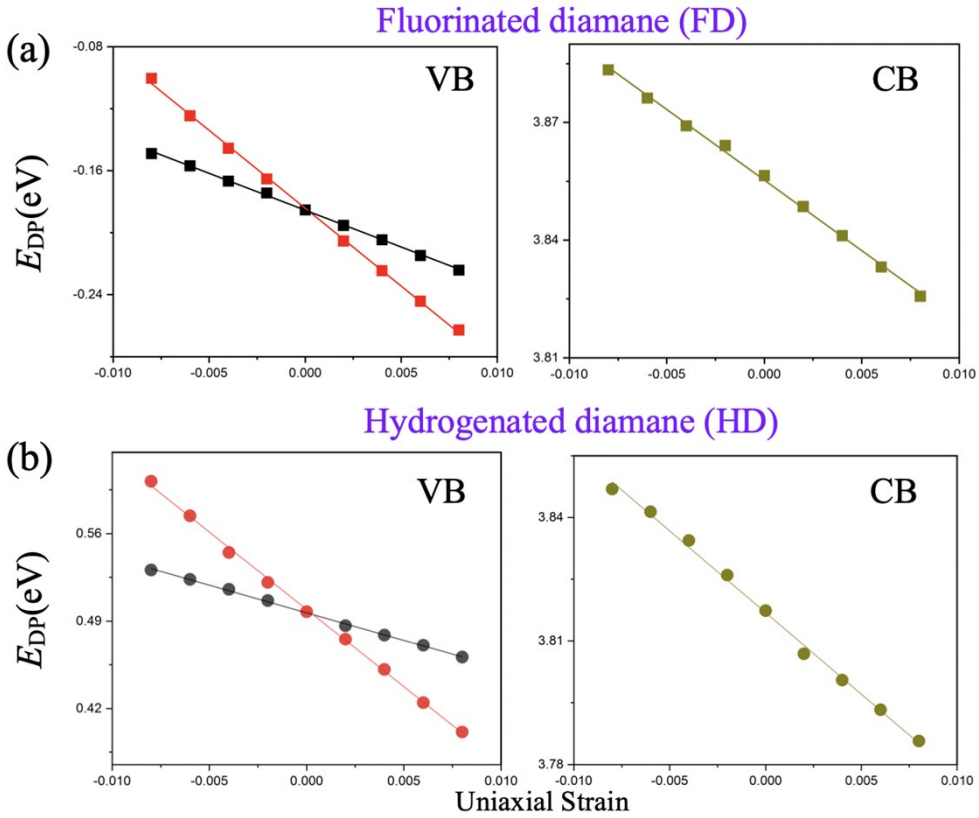

Figure S-4. Determination of the deformation potential constant E_1 for (a) FD and (b) HD. (left) Doubly degenerated Valence Band-edge energy as a function of applied uniaxial strains (right) Conduction Band-edge energy as a function of applied uniaxial strains.

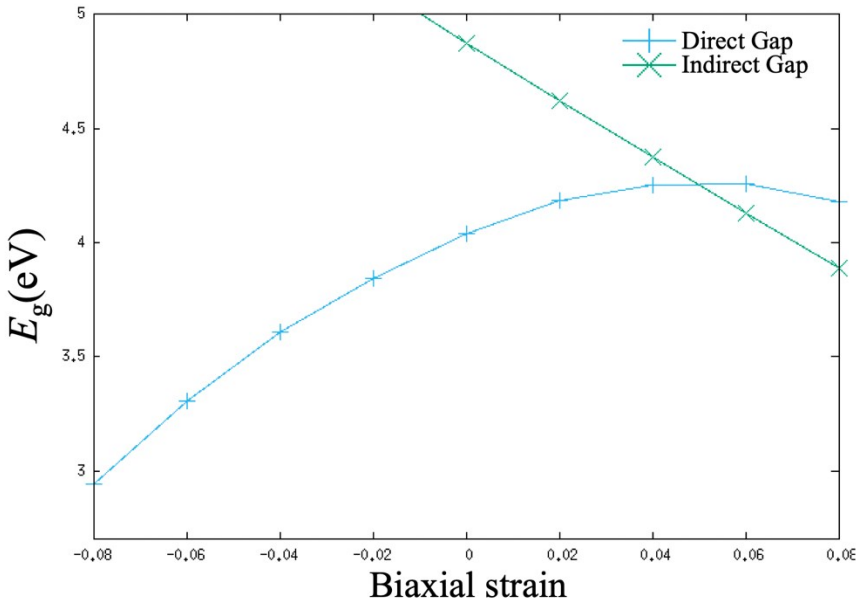

Figure S-5. The bandgap as a function of the applied biaxial strains for FD. The direct bandgap at Γ point under different strain is shown in blue symbol, while the indirect bandgap from Γ to M is shown in green symbol.

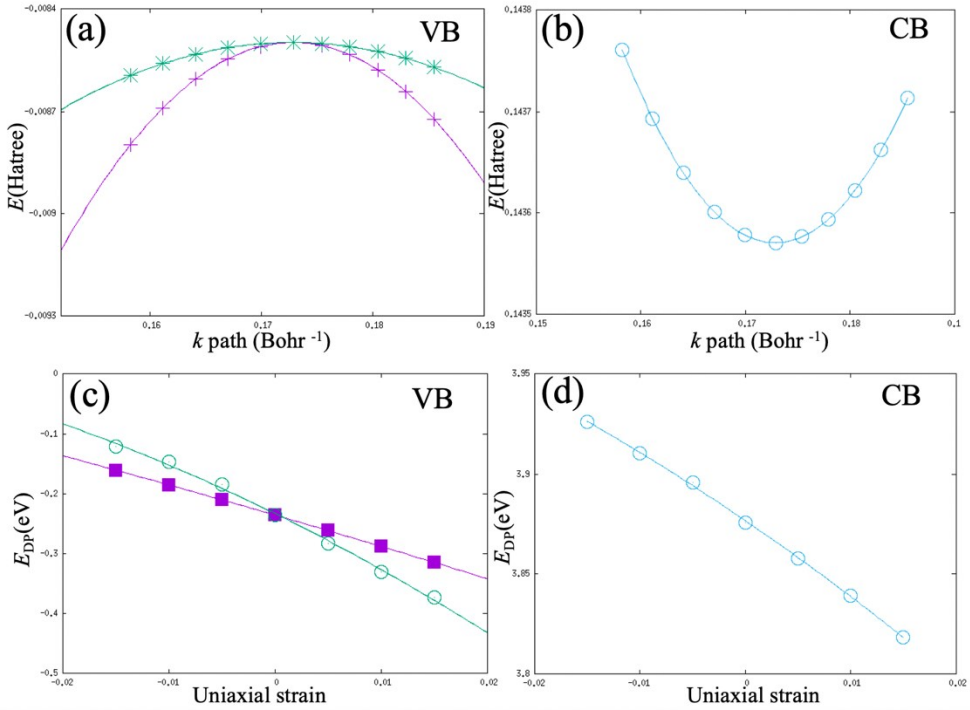

Figure S-6. Determination of the (a-b) effective mass and (c-d) deformation potential constant E_1 for FD 5×5 supercell with a single fluorine vacancy.

Table S-1 Effective masses (in electron mass me units) for FD and HD calculated using GW_0 and PBE method.

System	Method	VBM (hole)	CBM (electron)
		$m^*(m_e)$	$m^*(m_e)$
FD	PBE	1.13/0.37	0.55
	GW_0	1.05/0.31	0.60
HD	PBE	0.21/0.58	1.11
	GW_0	0.22/0.70	1.40