Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

for

Structural stability, electronic and mechanical properties of nitrogen and boron doped fluorinated diamane

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Table S1 Formation energies of pristine F-diamane and F-diamane with dopants.

structures	**formation energy (eV)**
F-diamane	-0.545
FD-1N	-0.528
FD-3N	-0.539
FD-1B	-0.539
FD-2B	-0.555
FD-3B	-0.533

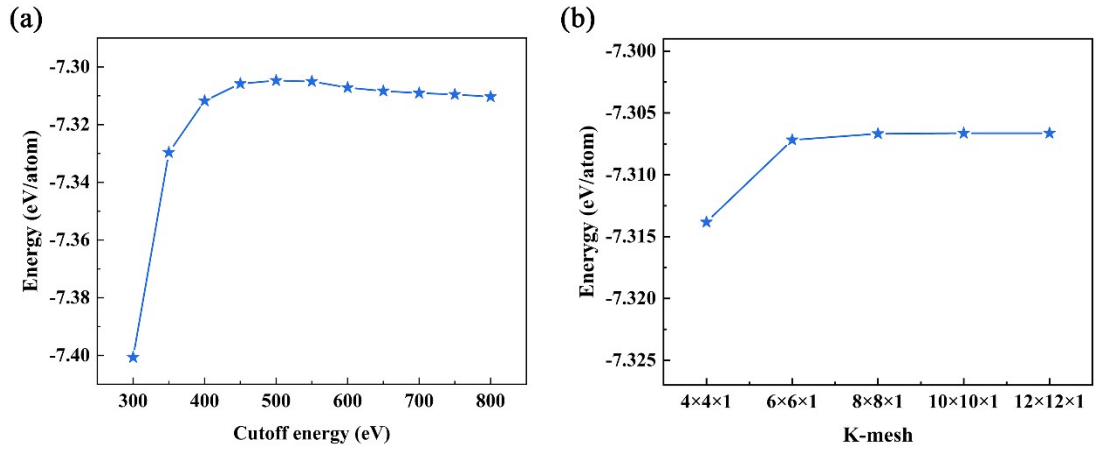

Fig. S1 Convergence test of plane wave cutoff energy and *k*-points.

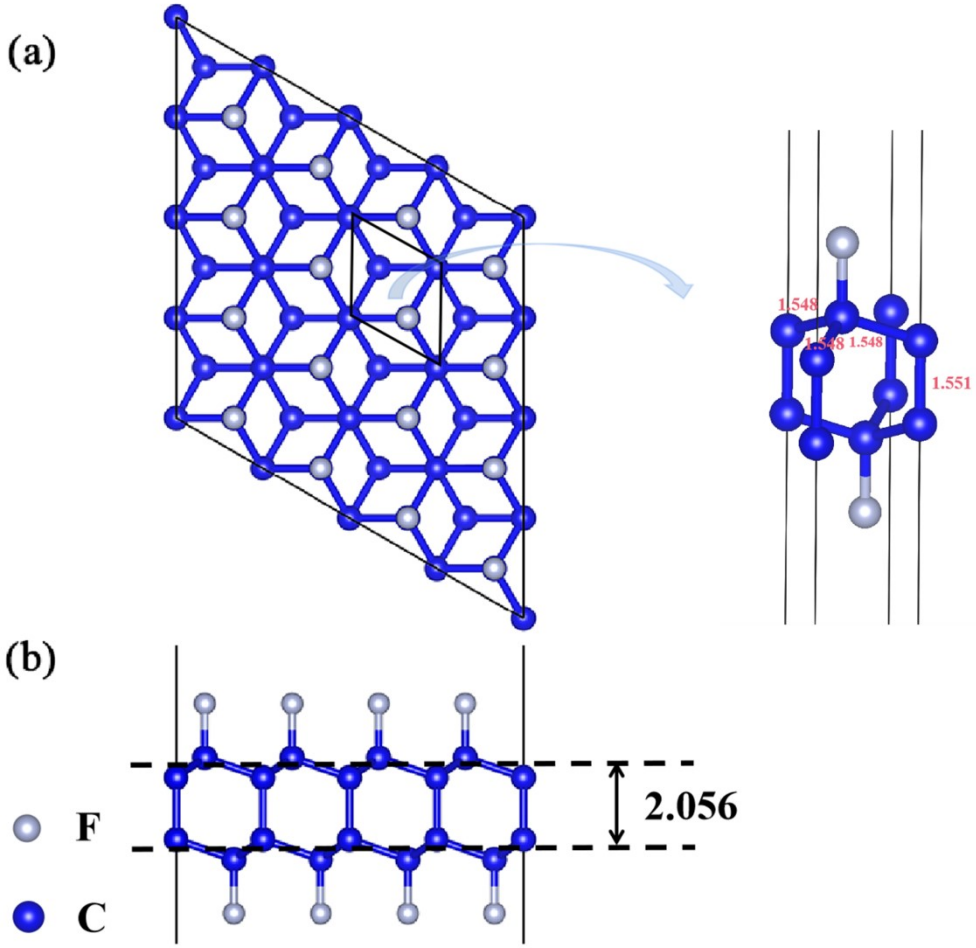

Fig. S2 (a) Top and (b) side views of F-diamane with 4×4×1 supercell. The interlayer separation and C-C bond lengths are labeled.

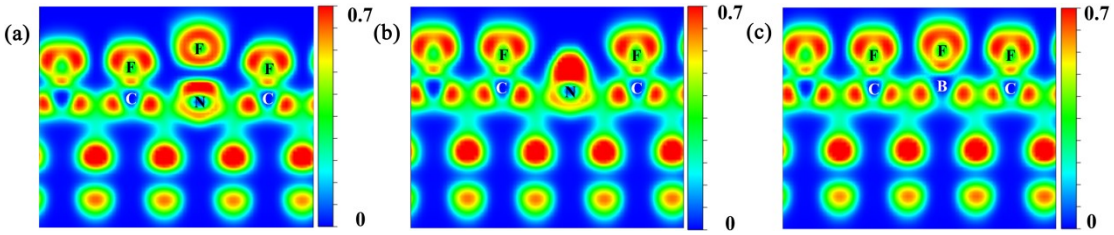

Fig. S3 Electron localization function of (a) FD-2N, (b) FD-3N and (c) FD-2B structures. The red (blue) regions represent the localized (delocalized) electronic states.

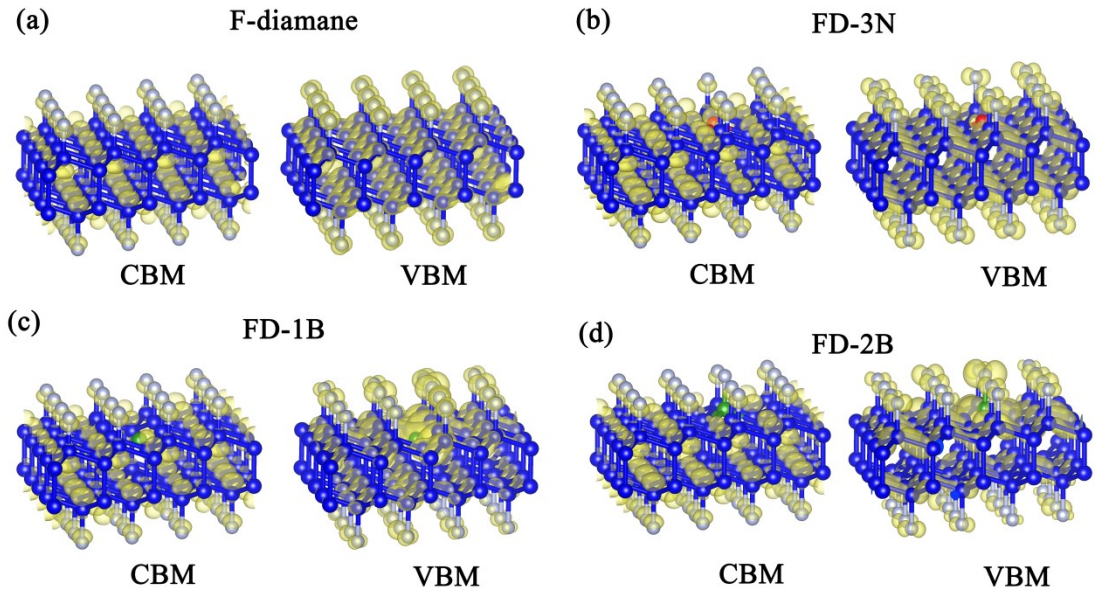

Fig. S4 Charge density of CBM and VBM at Γ point for (a) F-diamane, (b) FD-3N, (c) FD-1B, (d) FD-2B structures with an isosurface level of 0.002 e/Å^3.

CBM and VBM for FD-3N, FD-1B, FD-2B structures are nearly the same as pristine F-diamane, except the slight contribution of B dopants in VBM for FD-1B and FD-2B structures.