Supporting Information

for

Electronic structures of diamane doped with metal atoms

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Table S1 Interlayer separation *d* of F-diamane with different functionals and corrections.

		d (Å)
functional	PBE	2.054
	LDA	2.024
	HSE06	2.054
correction	DFT-D3	2.054
	DFT-D2	2.055
	OptB86b	2.054
	exp	2.05[1]

Reference:

(1) Bakharev, P. V.; Huang, M.; Saxena, M.; Lee, S. W.; Joo, S. H.; Park, S. O.; Dong, J.; Camacho-Mojica, D. C.; Jin, S.; Kwon, Y.; et al. Chemically induced transformation of chemical vapour deposition grown bilayer graphene into fluorinated single-layer diamond. *Nat. Nanotechnol.* **2020**, *15* (1), 59-66. DOI: 10.1038/s41565-019-0582-z.

Table S2 Bond length of metal atom and carbon atom $d_{M\text{-}C}$, binding energy E_b, and cohesive energy E_{coh} for diamane with metal atom absorption (M-$C_{64}H_{31}$ and M-$C_{64}F_{31}$).

	M-$C_{64}H_{31}$			M-$C_{64}F_{31}$		
	$d_{M\text{-}C}$ (Å)	E_b (eV)	E_{coh} (eV)	$d_{M\text{-}C}$ (Å)	E_b (eV)	E_{coh} (eV)
Li	2.08	-1.59	-1.66	2.07	-3.98	-1.66
Na	2.42	-1.24	-1.20	2.41	-3.56	-1.20
Mg	2.34	-1.09	-1.76	2.26	-2.27	-1.76
Al	2.09	-2.78	-3.67	2.37	-3.78	-3.67
K	2.76	-1.12	-0.95	2.80	-3.84	-0.95
Ca	2.42	-1.53	-2.05	2.42	-3.62	-2.05
Ti	2.19	-2.40	-5.80	2.20	-3.67	-5.80
V	2.52	-1.99	-5.89	2.17	-3.27	-5.89
Cr	2.12	-1.88	-4.47	2.21	-2.66	-4.47
Mn	2.37	-1.62	-4.13	2.31	-2.62	-4.13
Fe	2.05	-2.28	-5.21	1.99	-2.48	-5.21
Co	1.99	-2.41	-5.26	1.96	-3.06	-5.26
Ni	1.95	-3.07	-5.52	1.93	-4.06	-5.52
Cu	1.97	-2.60	-3.97	1.96	-2.81	-3.97
Zn	2.36	-0.74	-1.57	2.18	-0.98	-1.57
Pd	2.07	-2.32	-4.25	2.11	-2.43	-4.25
Ag	2.23	-1.93	-2.95	2.29	-2.17	-2.95
Pt	2.05	-3.49	-6.21	2.03	-2.85	-6.21
Au	2.15	-2.78	-3.61	2.16	-1.79	-3.61

Table S3 Bond length of metal atom with carton atom, binding energy E_b and cohesive energy E_{coh} for diamane with metal atom embedding (M-$C_{63}H_{31}$ or M-$C_{63}F_{31}$).

	M-$C_{63}H_{31}$			M-$C_{63}F_{31}$		
	d_{M-C} (Å)	E_b (eV)	E_{coh} (eV)	d_{M-C} (Å)	E_b (eV)	E_{coh} (eV)
Li	2.06	-1.67	-1.66	2.50	-3.89	-1.66
Na	2.43	-0.60	-1.20	2.94	-3.69	-1.20
Mg	2.25	-0.45	-1.76	2.24	-3.39	-1.76
Al	1.82	-2.27	-3.67	1.92	-5.15	-3.67
K	2.75	-0.76	-0.95	3.52	-4.05	-0.95
Ca	2.32	-1.86	-2.05	2.55	-5.81	-2.05
Ti	2.01	-5.54	-5.80	2.14	-7.96	-5.80
V	1.97	-4.81	-5.89	2.06	-6.94	-5.89
Cr	1.94	-3.98	-4.47	2.01	-6.02	-4.47
Mn	1.90	-3.80	-4.13	1.95	-5.11	-4.13
Fe	1.86	-4.90	-5.21	1.89	-6.10	-5.21
Co	1.82	-5.89	-5.26	1.86	-6.96	-5.26
Ni	1.89	-5.19	-5.52	1.91	-6.26	-5.52
Cu	1.91	-2.07	-3.97	1.99	-3.55	-3.97
Zn	2.14	0.37	-1.57	2.03	-1.11	-1.57
Pd	2.03	-3.29	-4.25	2.05	-4.14	-4.25
Ag	2.46	-0.24	-2.95	2.38	-1.81	-2.95
Pt	2.03	-5.30	-6.21	2.03	-5.33	-6.21
Au	2.26	-1.00	-3.61	2.20	-1.25	-3.61

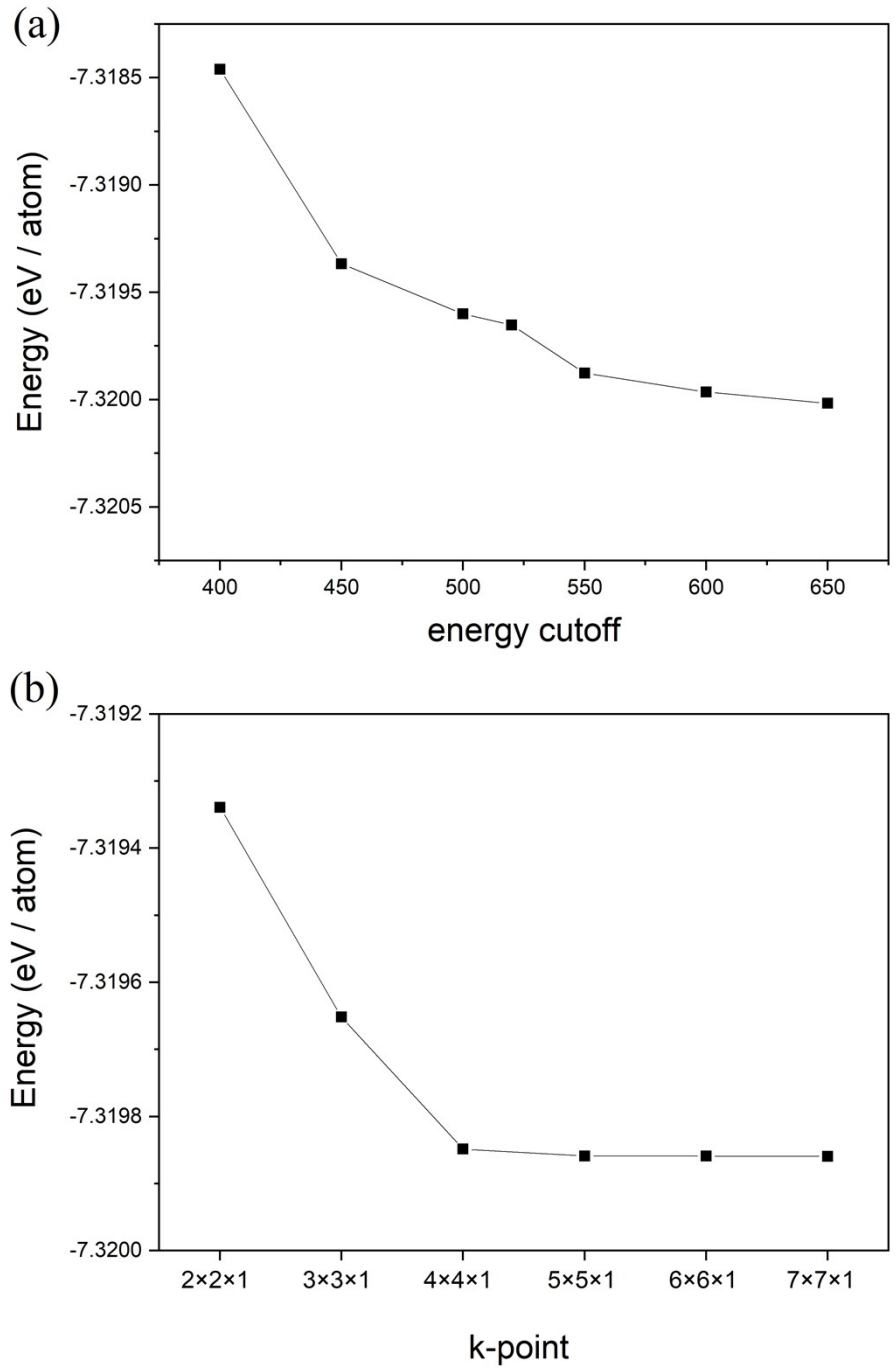

Figure S1. (a) Energy cutoff convergence test of sampling densities ranged from 400 to 650 eV, (b) *k*-point convergence test of sampling densities ranged from 2×2×1 to 7×7×1 for Li-$C_{64}H_{31}$ as an example.

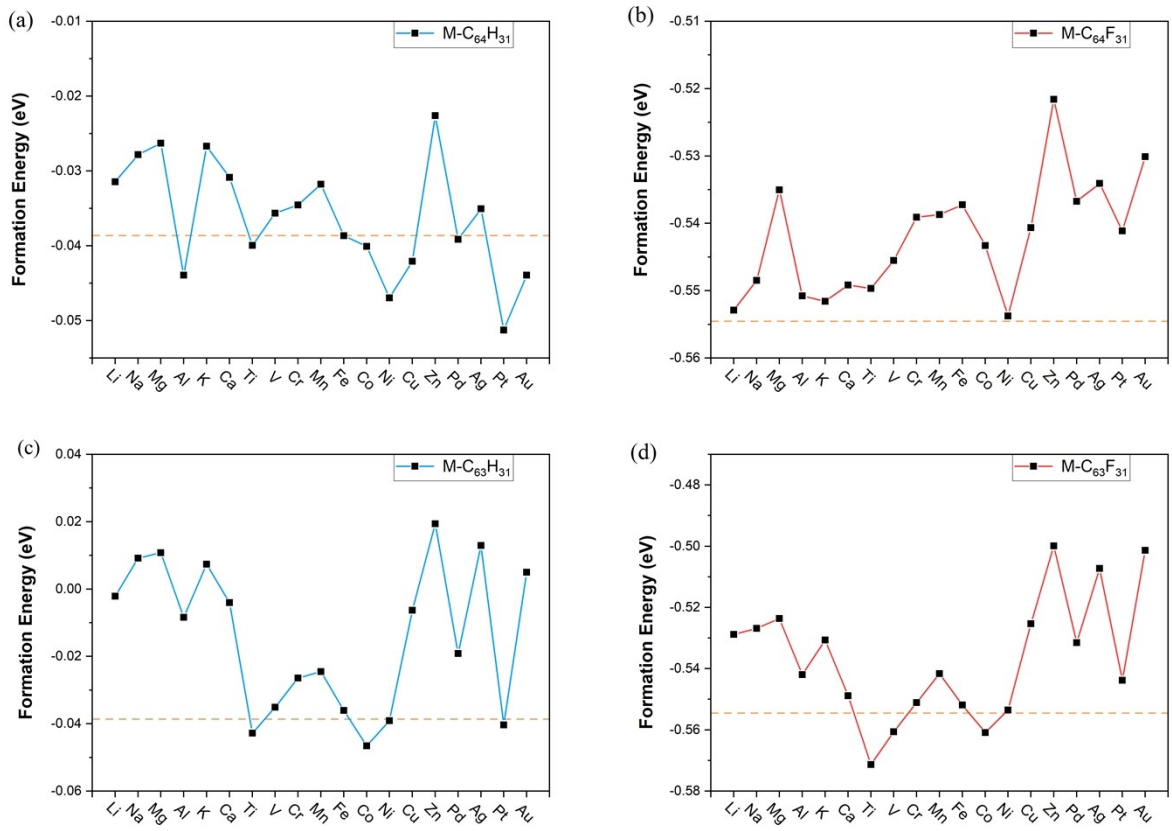

Figure S2. Formation energy (E_F) for (a) M-$C_{64}H_{31}$, (b) M-$C_{64}F_{31}$, (c) M-$C_{63}H_{31}$ and (d)M-$C_{63}F_{31}$. The dashed yellow lines represent the formation energy values of H-diamane or F-diamane without metal atoms.

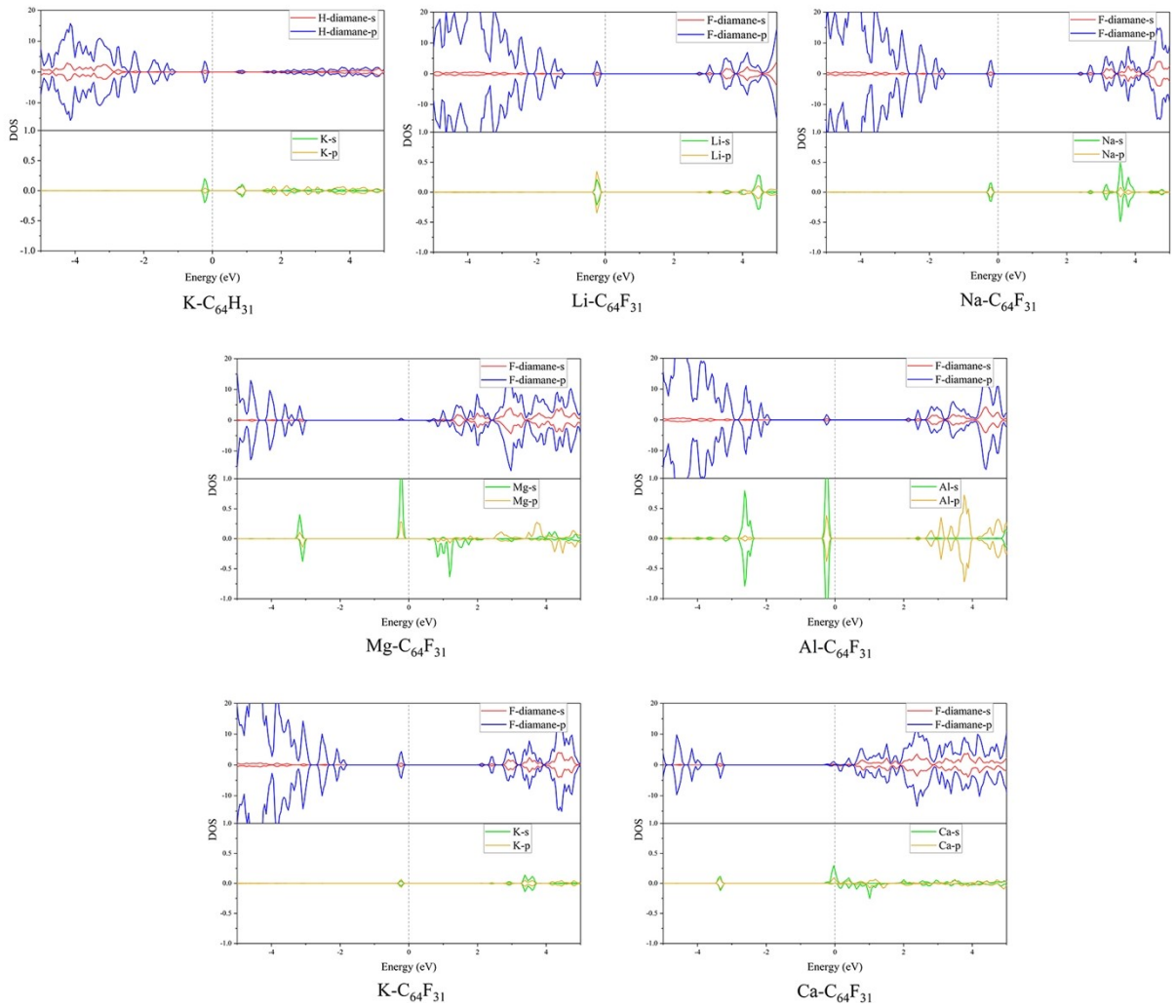

Figure S3. Density of states for diamane with metal atom absorption (M-$C_{64}H_{31}$ and M-$C_{64}F_{31}$). The Fermi level is set at zero.

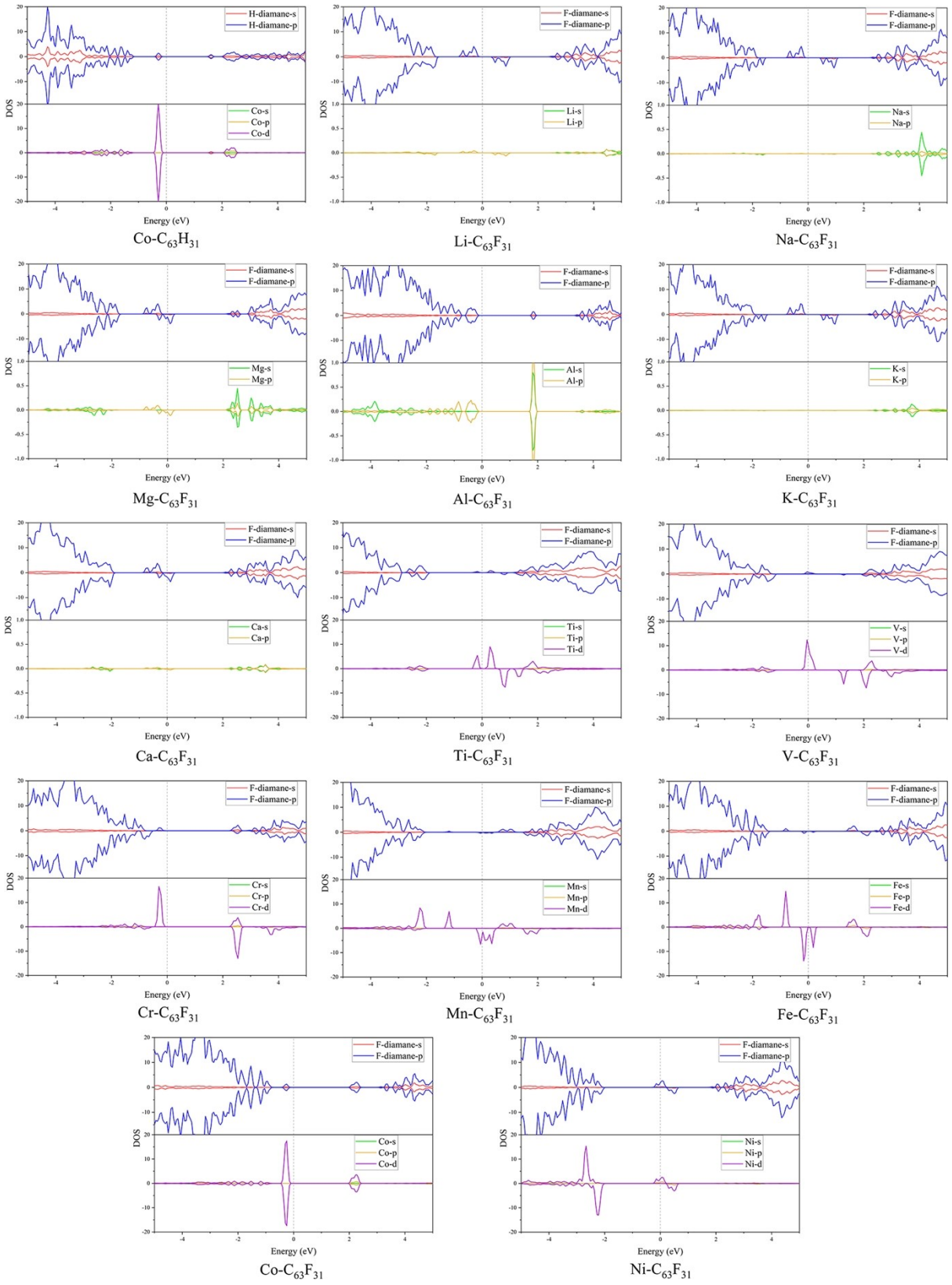

Figure S4. Density of states for diamane with metal atom embedding (M-$C_{63}H_{31}$ or M-$C_{63}F_{31}$). The Fermi level is set at zero.

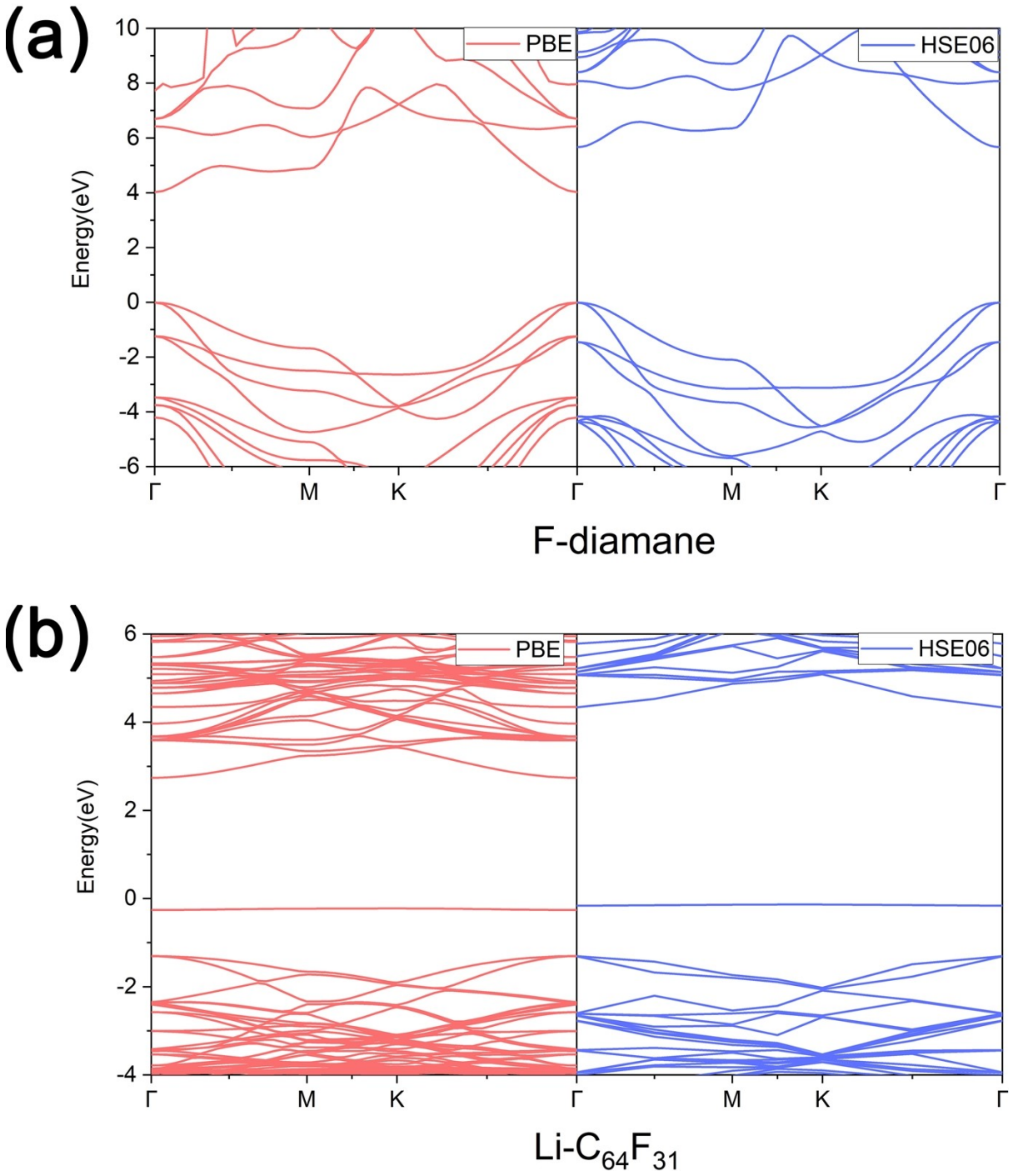

Figure S5. Band structures of (a) F-diamane, (b) Li-$C_{64}F_{31}$ calculated by PBE and HSE06 functionals.

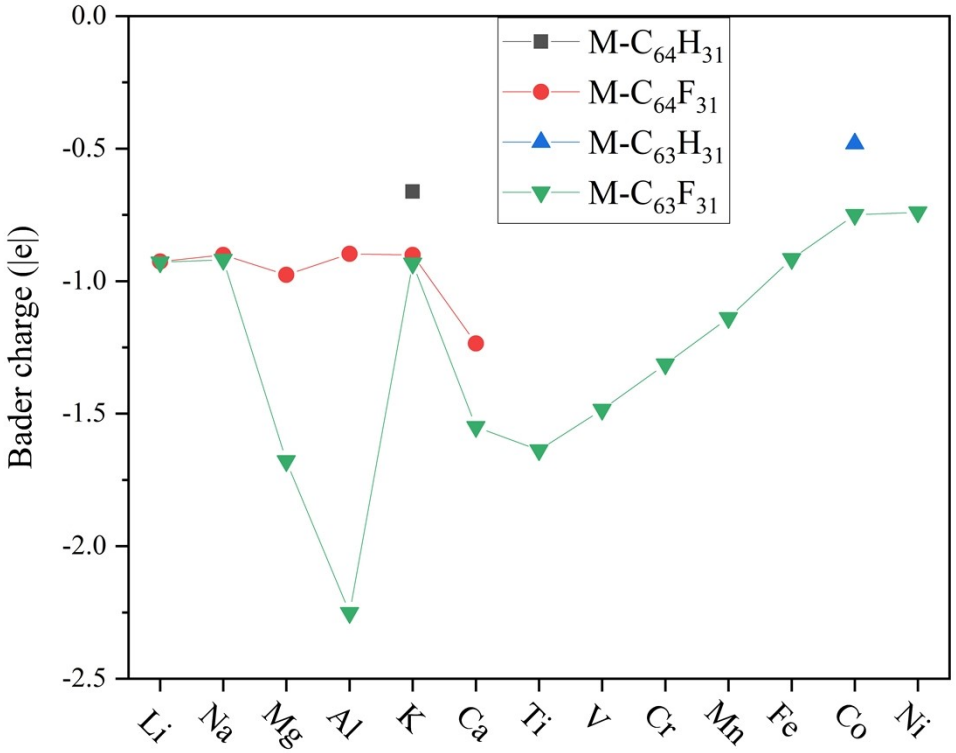

Figure S6. Bader charge values for diamane with metal atom doping and embedding.