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Supplementary Information

Non-covalent Interactions for Carbonaceous Materials: Impacts of Doping, Curving and their Combination

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Table S1. Combined effects (Ω) during NaF adsorption onto the outer and inner surfaces of doped graphene flakes with different curvatures (D-cGFs), calculated at B3LYP/bs1 level of theory.

dopant	ρ (nm^{-1})	Outer Surface		Inner surface	
		c_AGFo	c_ZGFo	c_AGFi	c_ZGFi
Be	0.492/0.491	8.1	9.7	40.3	65.5
	0.983/0.982	3.3	8.3	101.2	111.5
	1.475/1.503	-1.6	6.3	N.A. [a]	N.A. [a]
B	0.492/0.491	-10.6	-9.1	26.7	27.8
	0.983/0.982	-19.0	-17.1	N.A. [a]	N.A. [a]
	1.475/1.503	-27.7	-28.2	N.A. [a]	N.A. [a]
N	0.492/0.491	2.0	-0.6	-3.5	-0.7
	0.983/0.982	4.9	0.0	-7.8	-0.8
	1.475/1.503	6.9	0.3	-15.6	-2.2
O	0.492/0.491	9.2	6.3	-1.1	4.0
	0.983/0.982	12.3	7.1	-3.9	5.8
	1.475/1.503	14.5	6.3	-7.6	5.7

[a] The binding configuration is not geometrically stable.

Table S2. Combined effects (Ω) during NaF adsorption onto the outer and inner surfaces of doped graphene flakes with different curvatures (D-cGFs), calculated at M06-2X/bs2//B3LYP/bs1 level of theory.

dopant	ρ (nm^{-1})	Outer Surface		Inner surface	
		c_AGFo	c_ZGFo	c_AGFi	c_ZGFi
Be	0.492/0.491	14.3	16.4	36.6	62.3
	0.983/0.982	9.0	15.4	96.9	110.2
	1.475/1.503	4.1	16.5	N.A. [a]	N.A. [a]
B	0.492/0.491	-7.7	-6.8	21.4	22.0
	0.983/0.982	-18.2	-16.1	N.A. [a]	N.A. [a]
	1.475/1.503	-27.9	-26.7	N.A. [a]	N.A. [a]
N	0.492/0.491	1.8	0.3	-3.6	-0.9
	0.983/0.982	5.9	1.7	-9.4	-3.6
	1.475/1.503	8.8	3.6	-15.1	-6.3
O	0.492/0.491	16.8	14.7	-1.9	3.1
	0.983/0.982	20.7	17.9	-6.1	3.8
	1.475/1.503	23.0	19.3	-8.3	3.8

[a] The binding configuration is not geometrically stable.

Table S3. Combined effects (Ω) during NaF adsorption onto the outer and inner surfaces of doped graphene flakes with different curvatures (D-cGFs), calculated at cam-B3LYP/bs2//B3LYP/bs1 level of theory.

dopant	ρ (nm^{-1})	Outer Surface		Inner surface	
		c_AGFo	c_ZGFo	c_AGFi	c_ZGFi
Be	0.492/0.491	11.4	18.6	42.5	53.0
	0.983/0.982	6.0	18.0	106.2	112.3
	1.475/1.503	1.4	12.3	N.A. [a]	N.A. [a]
B	0.492/0.491	-5.7	-5.5	18.1	18.1
	0.983/0.982	-16.9	-16.1	N.A. [a]	N.A. [a]
	1.475/1.503	-26.6	-27.5	N.A. [a]	N.A. [a]
N	0.492/0.491	1.6	-0.8	-2.9	0.1
	0.983/0.982	4.8	0.1	-8.4	-1.6
	1.475/1.503	7.4	1.1	-15.1	-3.5
O	0.492/0.491	9.0	5.8	-2.6	2.9
	0.983/0.982	12.9	7.4	-6.6	4.1
	1.475/1.503	15.4	7.6	-10.0	4.3

[a] The binding configuration is not geometrically stable.

Table S4. Combined effects (Ω) during NaF adsorption onto the outer and inner surfaces of doped graphene flakes with different curvatures (D-cGFs), calculated at cam-B3LYP-D3/bs2//B3LYP/bs1 level of theory.

dopant	ρ (nm^{-1})	Outer Surface		Inner surface	
		c_AGFo	c_ZGFo	c_AGFi	c_ZGFi
Be	0.492/0.491	11.7	18.6	43.4	54.7
	0.983/0.982	6.0	17.4	104.7	110.7
	1.475/1.503	1.1	9.7	N.A. [a]	N.A. [a]
B	0.492/0.491	-5.9	-6.1	16.4	16.5
	0.983/0.982	-17.2	-16.9	N.A. [a]	N.A. [a]
	1.475/1.503	-26.8	-28.5	N.A. [a]	N.A. [a]
N	0.492/0.491	1.6	-0.6	-2.4	0.4
	0.983/0.982	5.4	0.8	-7.4	-0.8
	1.475/1.503	8.6	2.2	-9.2	-1.8
O	0.492/0.491	10.5	7.6	-2.3	3.2
	0.983/0.982	14.8	9.8	-5.7	4.5
	1.475/1.503	17.8	10.3	-7.9	4.6

[a] The binding configuration is not geometrically stable.

Table S5. Combined effects (Ω) during NaF adsorption onto the outer and inner surfaces of doped graphene flakes with different curvatures (D-cGFs), calculated at vdW-DF level of theory.

dopant	ρ (nm^{-1})	Outer Surface		Inner surface	
		c_AGFo	c_ZGFo	c_AGFi	c_ZGFi
Be	0.492/0.491	12.3	9.9	30.2	81.0
	0.983/0.982	6.8	1.1	84.3	98.2
	1.475/1.503	2.6	-0.7	N.A. [a]	N.A. [a]
B	0.492/0.491	-11.7	-8.9	32.2	34.1
	0.983/0.982	-17.3	-14.7	N.A. [a]	N.A. [a]
	1.475/1.503	-23.1	-22.8	N.A. [a]	N.A. [a]
N	0.492/0.491	3.3	0.7	-3.8	-0.8
	0.983/0.982	6.2	1.7	-10.6	-2.8
	1.475/1.503	9.2	3.3	-18.5	-4.8
O	0.492/0.491	14.2	12.2	0.9	4.9
	0.983/0.982	16.4	12.5	-4.0	4.4
	1.475/1.503	19.2	13.2	-7.9	3.9

[a] The binding configuration is not geometrically stable.