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Electronic Supplementary Information

Novel insights into L-cysteine adsorption on transition metal doped graphene: influences of the dopant and the vacancy

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Tab. S1 Mulliken spin population of magnetic MSV and MDV systems. (Unit: μ_B)

MSV	M_{total}	M_{TM}	MDV	M_{total}	M_{TM}

ScSV	0	0	ScDV	0.218	0.026
VSV	0.998	1.156	VDV	1.006	1.026
CrSV	2.002	2.435	CrDV	2.001	2.535
MnSV	2.992	2.819	MnDV	3.097	3.539
CoSV	0.985	0.293	CoDV	1.073	1.195
CuSV	1.001	0.275	CuDV	0.199	0.009

Tab. S2 Linking sites between l-cys and MGs.

MSV	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
S	S	S	S	S	S	S	S	S	S	S
O	Bi-O[a]	Bi-O	Bi-O	Bi-O	Bi-O	Bi-O	Bi-O	Bi-O	Bi-O	Bi-O
N	N	N	N	N	N	N	N	N	N	N
MDV	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
S	S;O=	S	S	S	S	S	S	S	S	S
O	Bi-O	Bi-O	O[b]	O	Bi-O	Bi-O	Bi-O	Bi-O	O	O
N	N	N	N	N	N	N	N	N	N	N

[a]: Bi-O denotes linking sites include O in OH and O in O=.

[b]: O denotes the linking site is O in OH.

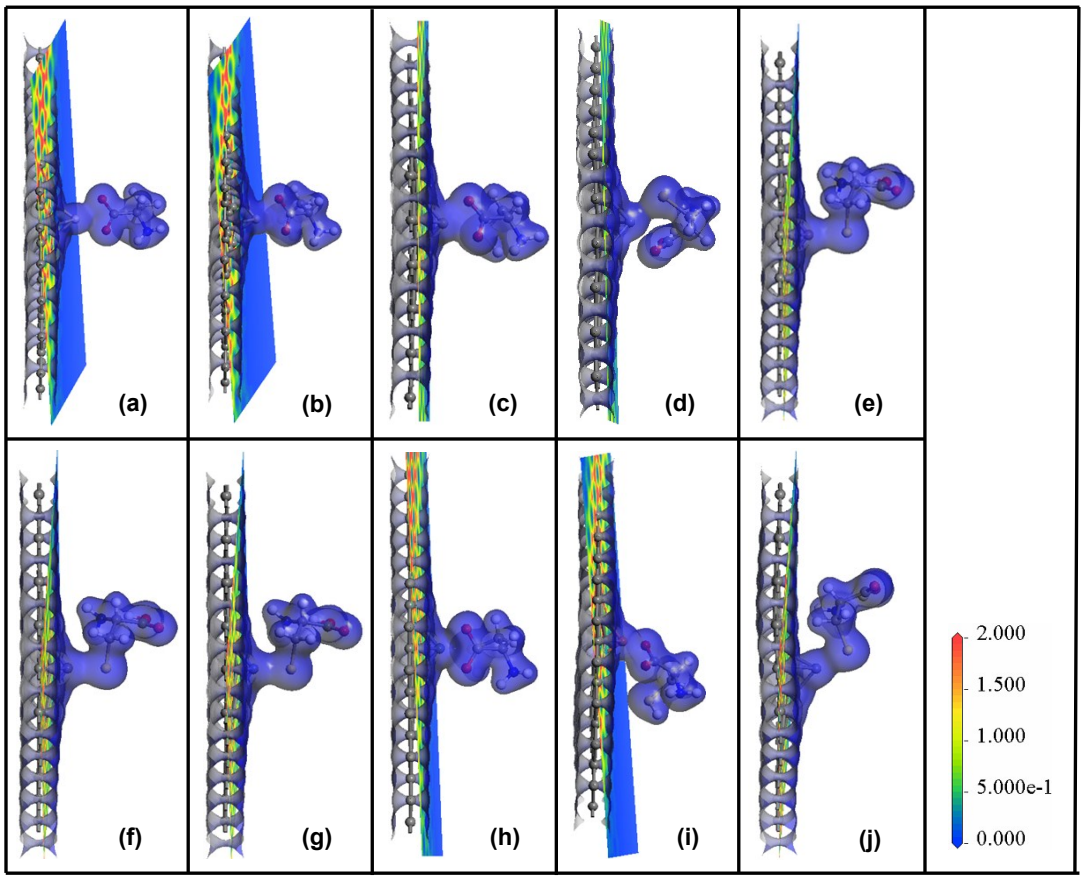

Fig. S1 Charge density graphs of the most stable adsorption on MSVs. (a) O-ScSV, (b) O-TiSV, (c) O-VSV, (d) S-CrSV, (e) S-MnSV, (f) S-FeSV, (g) S-CoSV, (h) O-NiSV, (i) O-CuSV and (j) S-ZnSV. The electrons are shown in a range of 0-2 e $Å^3$.

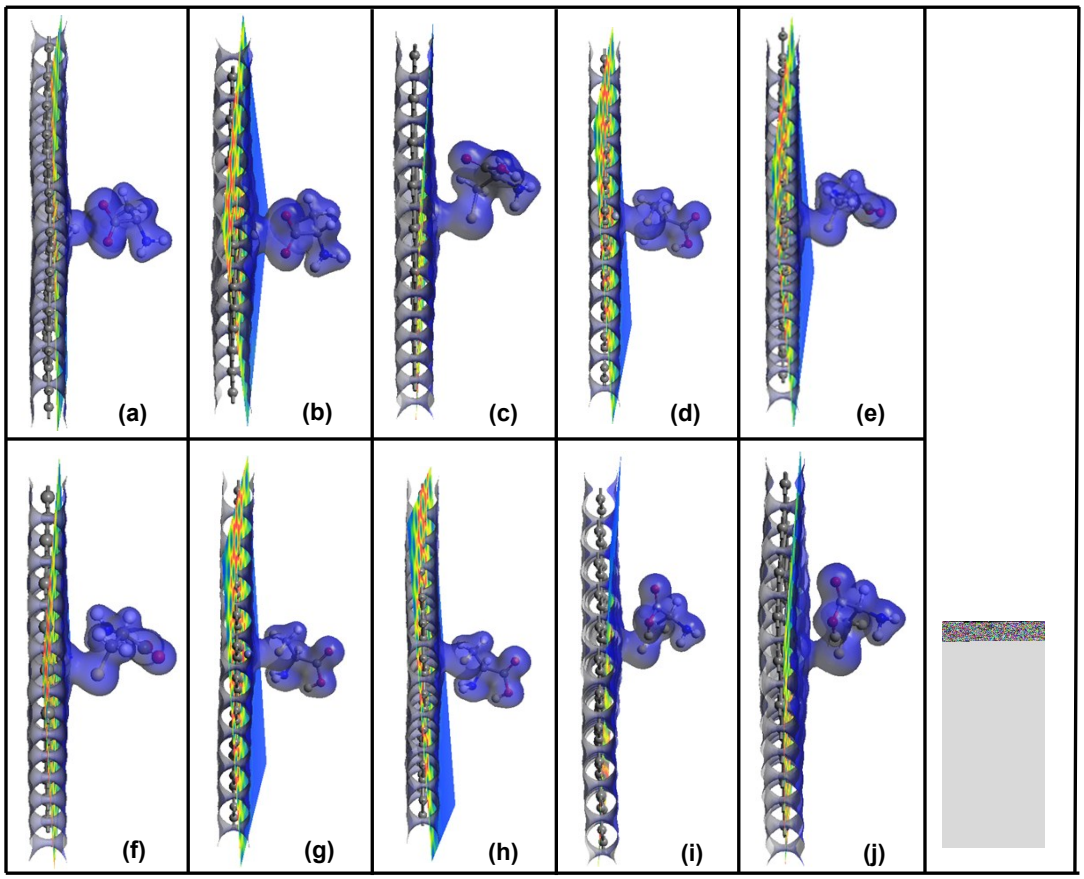

Fig. S2 Charge density graphs of the most stable adsorption on MDVs. (a) O-ScDV, (b) O-TiDV, (c) S-VDV, (d) S-CrDV, (e) S-MnDV, (f) S-FeDV, (g) S-CoDV, (h) S-NiDV, (i) S-CuDV and (j) S-ZnDV. The electrons are shown in a range of 0-2 e $Å^3$.

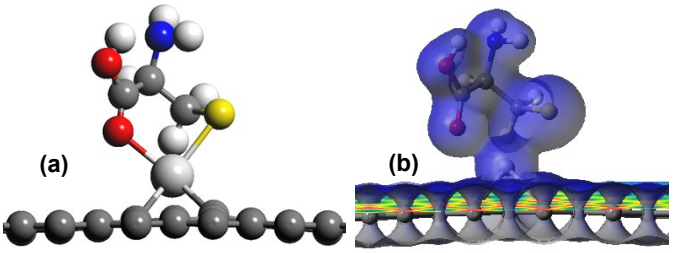

Fig. S3 Adsorption geometry (a) and charge density distribution (b) of S-ScDV. The electrons are shown in a range of 0-2 e Å^3.

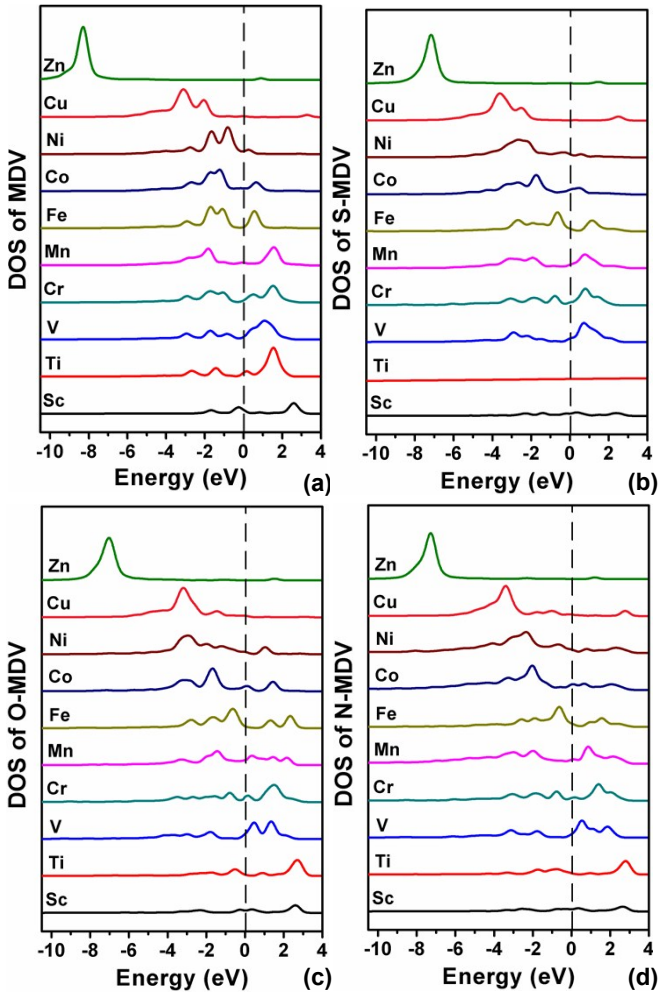

Fig. S4 Partial density of states (DOS) of the 3d orbital of the TM dopant in MDV (a), S-MDV (b), O-MDV (c) and N-MDV (d).

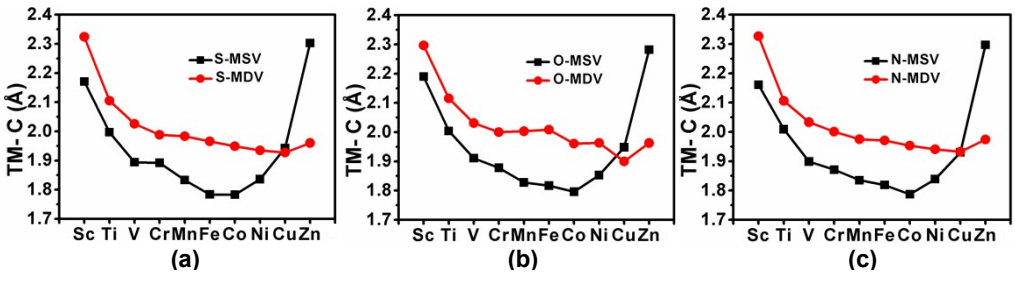

Fig. S5 The TM-C bond lengths of (a) S-MG, (b) O-MG and (c) N-MG adducts.

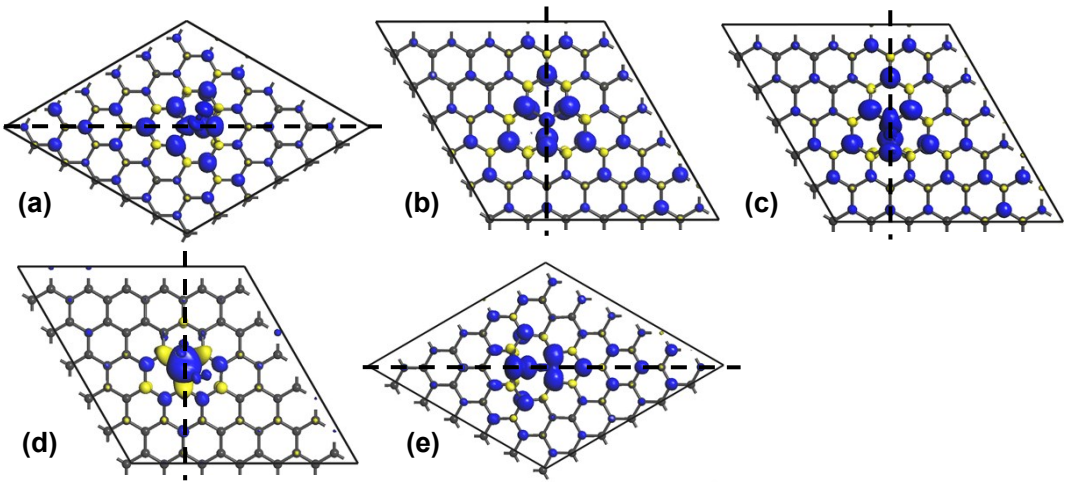

Fig. S6 Top views of spin density distributions on graphenes in S-NiSV (a), O-NiSV (b), N-NiSV(c), O-FeSV (d) and N-ZnSV (e). The isovalue is 0.01 e Å^3. The l-cys atoms were removed to illustrate the spin distribution on the MSV surface. The light yellow and dark blue surfaces correspond to majority and minority spins, respectively. The dashed line indicates the mirror line.

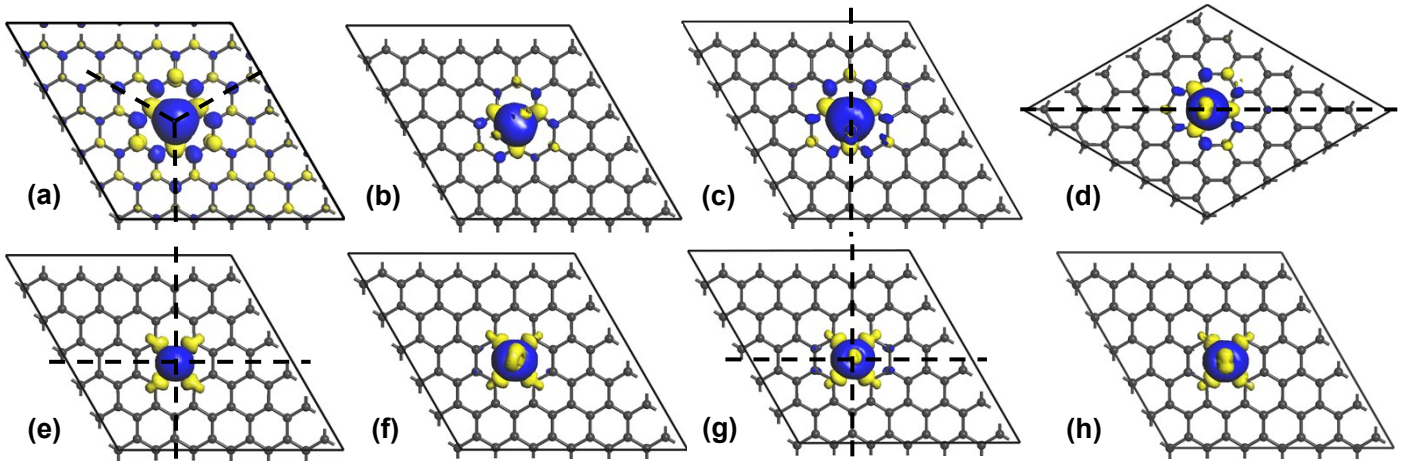

Fig. S7 Top views of spin density distributions on graphenes in CrSV (a), S-CrSV (b), O-CrSV(c), N-CrSV (d) and CrDV (e), S-CrDV (f), O-CrDV (g), N-CrDV (h). The isovalue is 0.01 e Å^3. The l-cys atoms in (b-d) and (f-h) were removed to illustrate the spin distribution on the MDV surface. The light yellow and dark blue surfaces correspond to majority and minority spins, respectively. The dashed line indicates the mirror line.

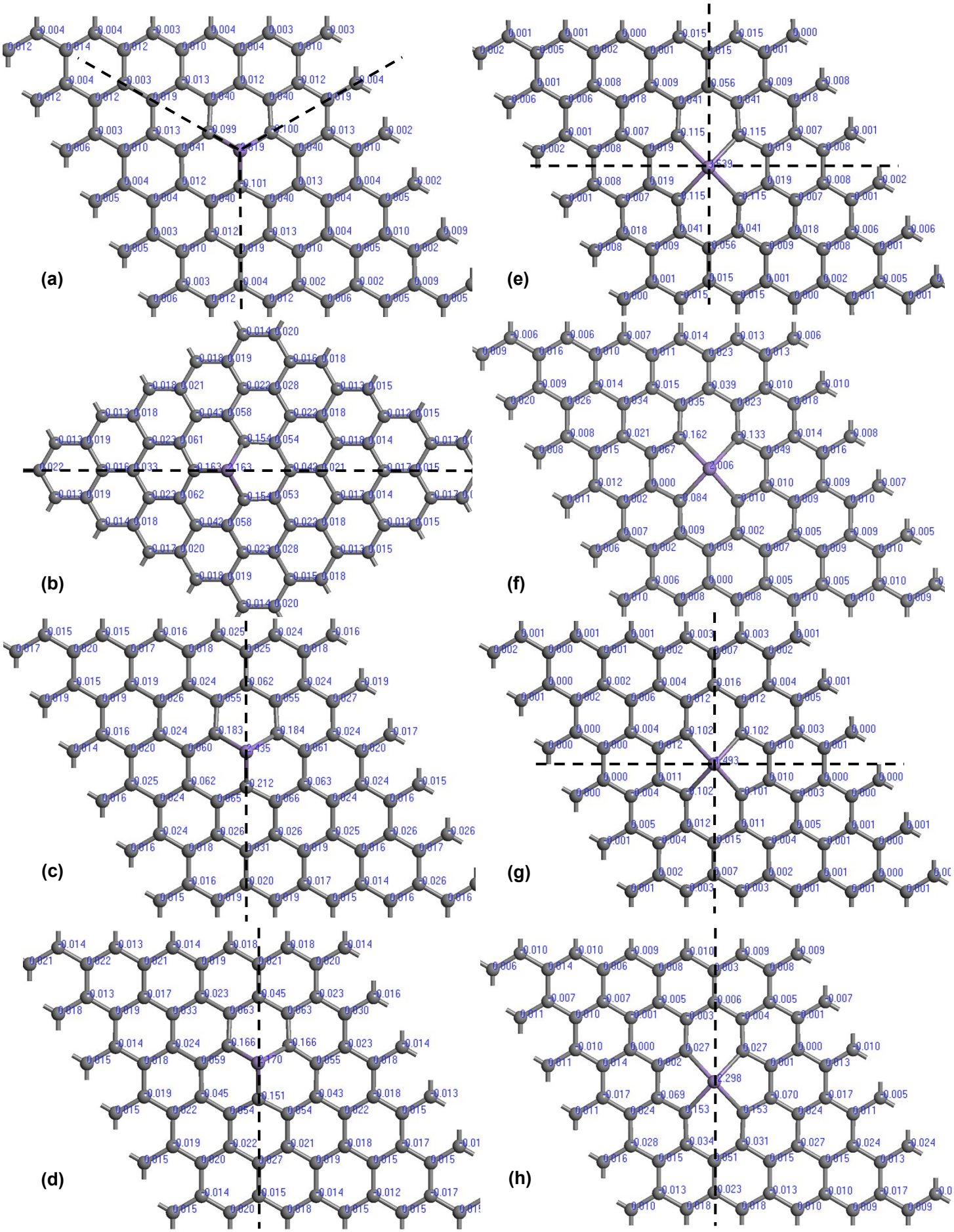
(a)
(b)
(c)
(d)
(e)
(f)
(g)
(h)

Fig. S8 Mulliken spin population of the (a) MnSV, (b) S-MnSV, (c) O-MnSV, (d) N-MnSV and (e) MnDV, (f) S-MnDV, (g) O-MnDV, (h) N-MnDV systems, where atoms of l-cys were removed to illustrate the spin distribution on the MnG surface.