

Supplementary information (SI)

Unravelling the Selective Transport of Co^{2+} and Hg^{2+} Ions through Functionalized Graphene Nanostructures from Aqueous Nitrate Solution: A Molecular Dynamics Simulation Study

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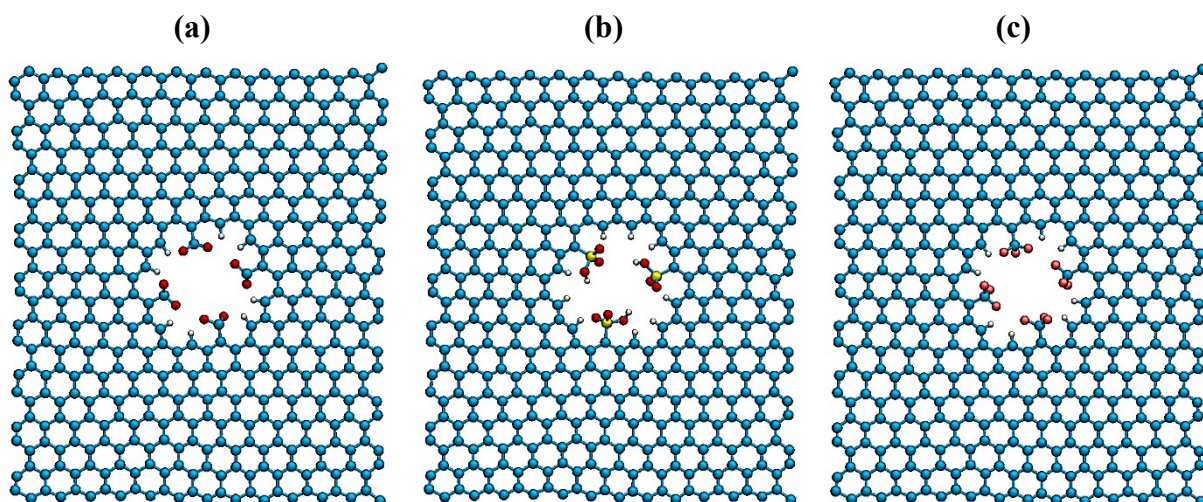


Fig. S1 Snapshots of nanoporous GRA membrane functionalized with (a) $-\text{COO}^-$, (b) $-\text{SO}_3\text{H}$, and (c) $-\text{CF}_3$. Carbon, oxygen, hydrogen, sulphur, and fluorine are represented by cyan, red, white, yellow, and pink colors respectively.

Table S1 List of non-bonding parameters

Molecules/Ions	Site	Charge (e)	$\sigma(\text{\AA})$	$\epsilon(\text{kcal/mol})$
COO^- -GRA	C(GRA)	0.1000	3.4000	0.0860
	C	0.7000	3.7500	0.1090
	O(C-O)	-1.0000	2.9600	0.2100
	O(C=O)	-0.8000	2.9600	0.2100
SO_3H -GRA	C(GRA)	-0.0134	3.5418	-0.0700
	S	1.4177	3.5418	-0.2500
	O(S=O)	-0.5636	2.9531	-0.1700
	O(S-O)	-0.7151	3.1127	-0.1700
	H	0.5316	0.0000	-0.0000
CF_3 -GRA	C(GRA)	-0.2042	3.5418	-0.0700
	C	0.4966	3.4919	-0.0660
	F	-0.1685	2.8933	-0.0600