

Supporting Information

Graphene oxide promoted cadmium uptake by rice in soil

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Table S1. 12-6 Lennard-Jones potential parameters and atomic charges used in the OPLS for graphene, carboxylate groups on graphene edges, and the Cd(II) ion. C₀, C₁ and C₂ denote carbon atoms in the *sp*² region of graphene, the carboxylate group, and the atom bonded to C₁.

	Atomic site	ϵ (kcal/mol)	σ (nm)	q (e)	Bond length (nm)
Graphene	C ₀	0.068	0.34	0	$l_{C-C} = 0.142$
Carboxylate	C ₁ (in COO ⁻)	0.105	0.375	0.7	$l_{C_1-O} = 0.125$ $l_{C_1-C_2} = 0.1522$
	O	0.21	0.296	-0.8	
	C ₂ (in graphene)	0.068	0.34	-0.1	
Water	H	0	0	0.4236	$l_{O-H} = 0.1$
	O	0.155	0.317	-0.8472	
Cd(II)	Cd	0.00848	0.2394	+2	/

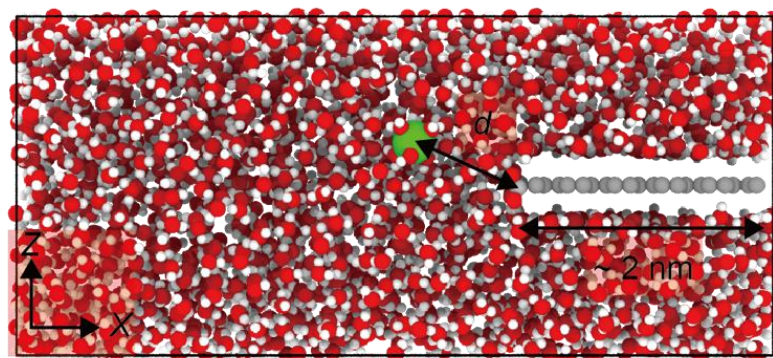


Figure S1. The MD simulation model.

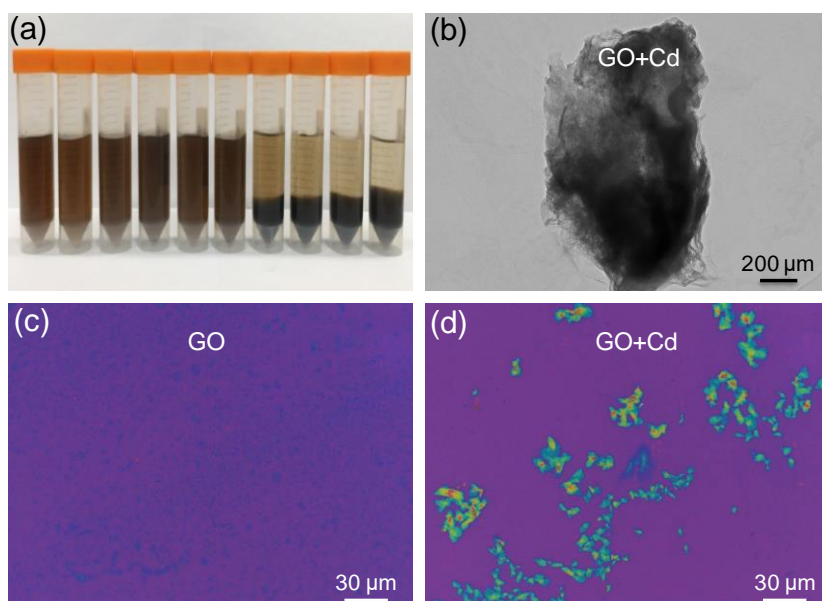


Figure S2. (a) Bulk aggregations of GO in solutions with varied initial Cd(II) concentration (5, 10, 15, 20, 25, 30, 35, 40, 45 and 50 mg/L). (b) TEM image of aggregated GO in the solution (initial Cd(II) concentration: 50 mg/L). (c, d) Optical images of GO and aggregated GO in the solution (initial Cd(II) concentration: 50 mg/L).

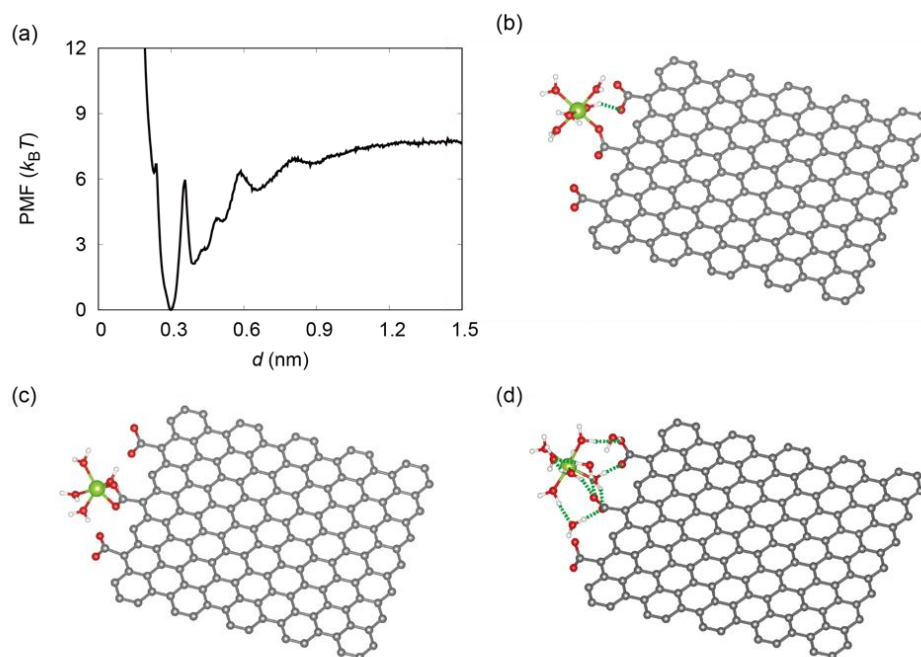


Figure S3. (a) PMF calculated from MD simulations. (b-d) Atomic structures illustrating absorption of hydrated Cd(II) at carboxylate groups, which occurs while the ion is trapped at (b) single or (c) double O atoms of carboxylate groups, or (d) mediated by H-bonds (the green dash lines) between water molecules on the 1HS of ions and the oxygen-containing groups. The atoms in water are shown in red (O) and white (H) surrounding the Cd(II) ions (green). The interaction between the water molecules in the 1HS and the ion is indicated by solid lines.

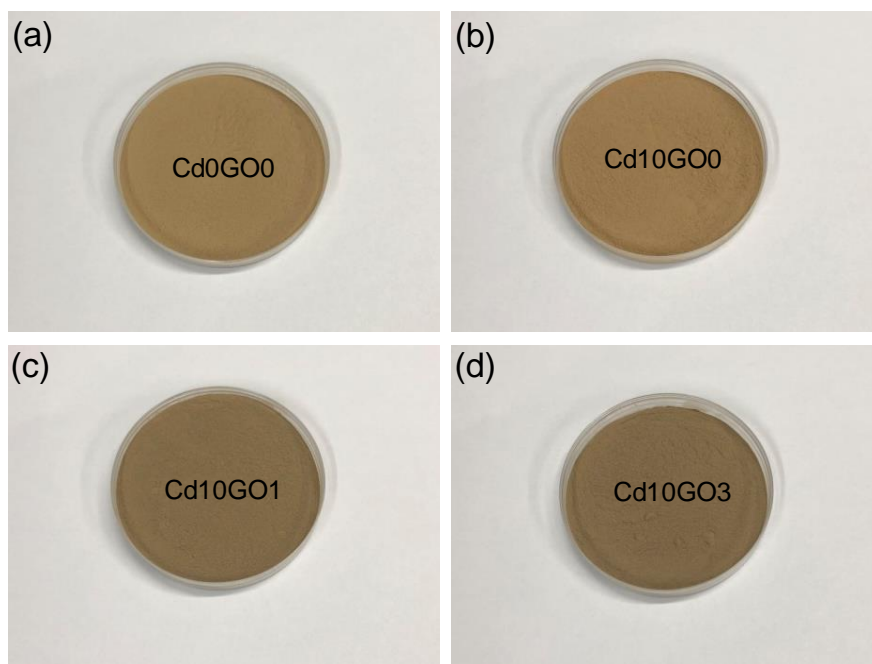


Figure S4. Photographs of soils treated with GO of different concentrations.