

SUPPLEMENTARY INFORMATION FOR:

Comparative Study of the Sorption Mechanism of Reactive Black 5 Dye on Raw and Carbonized Sorbent Derived from Industrial Hemp Biowaste

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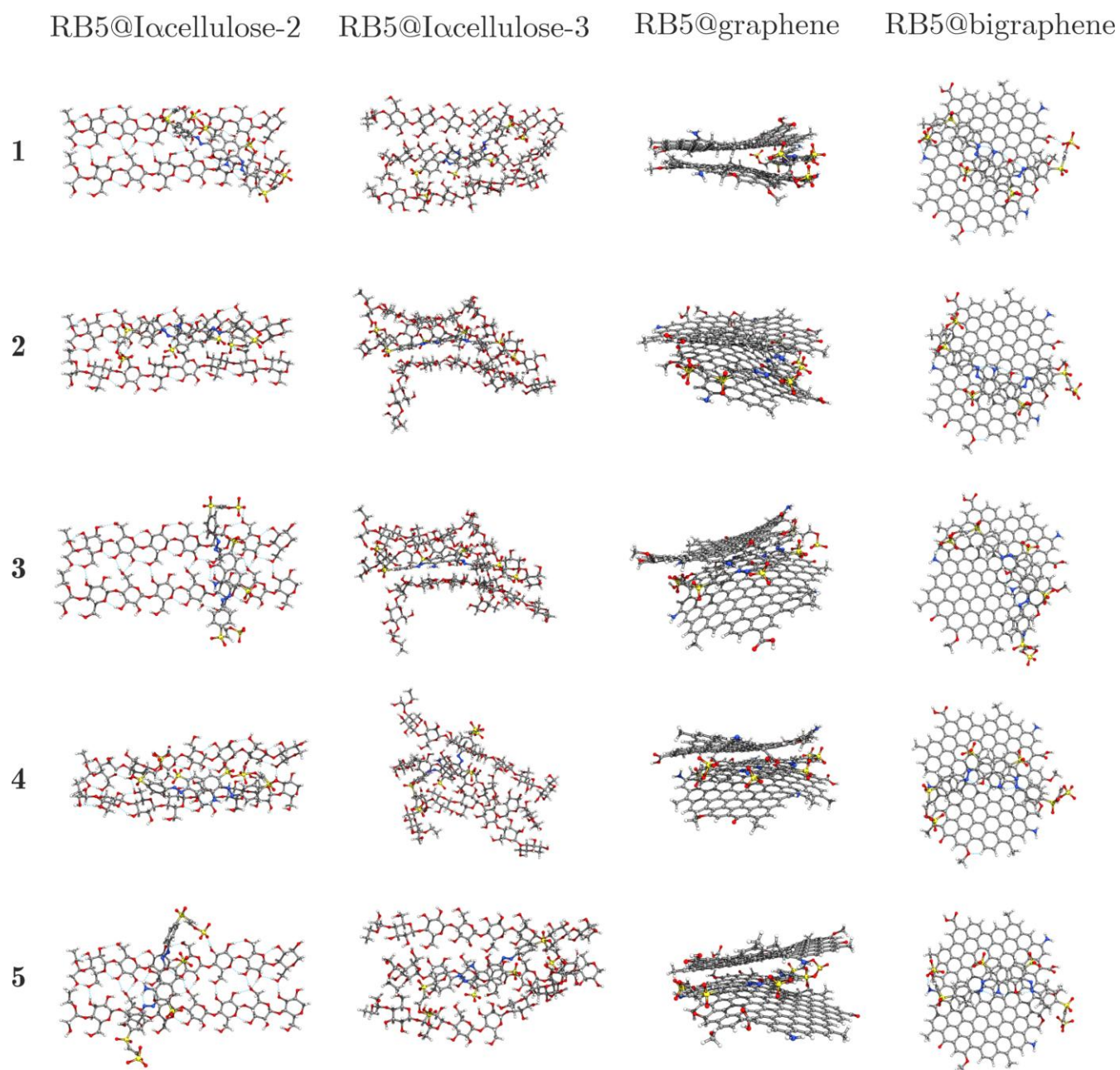


Figure S1. Five most stable optimized conformers of RB5 adsorbed on the investigated lignocellulosic and carbonized model systems: RB5@I α -cellulose-2, RB5@I α -cellulose-3, RB5@graphene and RB5@bigraphene.

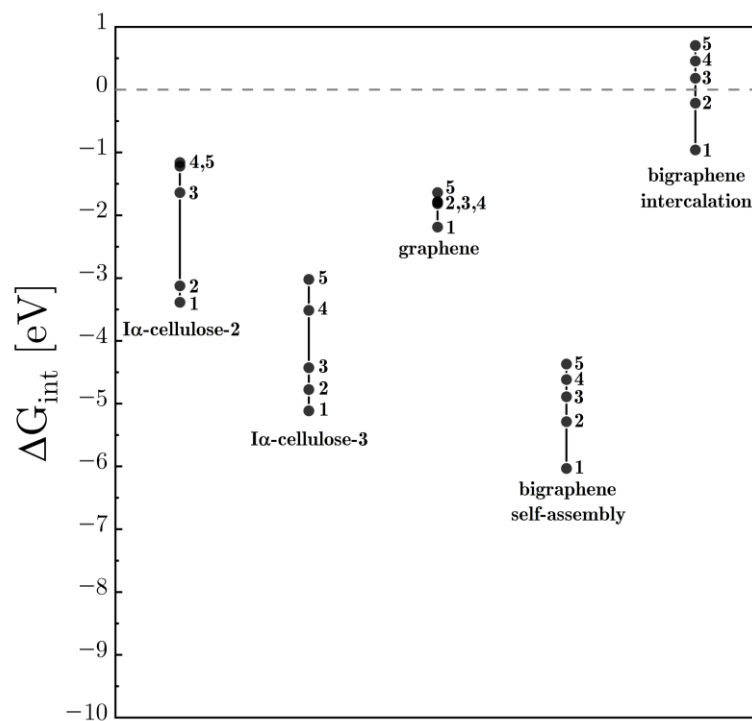


Figure S2. Calculated Gibbs free energies (eV) for the five lowest-energy conformers of RB5 adsorbed on lignocellulosic and carbonized model systems: RB5@I α -cellulose-2, RB5@I α -cellulose-3, RB5@graphene and RB5@bigraphene. See main text for explanation.

Table S1. Interaction energies (ΔE_{int} , eV) and Gibbs free energies (ΔG_{int} , eV) calculated at the GFN2-xTB level for the five lowest-energy conformers of RB5 adsorbed on lignocellulosic and carbonized model systems. Gibbs free energies include thermal and entropic corrections obtained within the RRHO approximation and implicit GBSA solvation model. Values are reported to illustrate relative stability trends across the different adsorption motifs.

	RB5@I α -cellulose-2		RB5@I α -cellulose-3		RB5@graphene		RB5@bigraphene self-assembly		RB5@bigraphene intercalation	
	ΔE_{int}	ΔG_{int}	ΔE_{int}	ΔG_{int}	ΔE_{int}	ΔG_{int}	ΔE_{int}	ΔG_{int}	ΔE_{int}	ΔG_{int}
1	-4.72	-3.39	-6.53	-5.11	-3.25	-2.19	-8.52	-6.03	-2.18	-0.96
2	-4.52	-3.12	-6.25	-4.78	-2.88	-1.82	-7.65	-5.29	-1.32	-0.22
3	-2.90	-1.64	-5.82	-4.43	-2.86	-1.80	-7.19	-4.89	-0.85	0.18
4	-2.24	-1.22	-4.78	-3.51	-2.81	-1.78	-6.86	-4.62	-0.52	0.46
5	-2.21	-1.16	-4.32	-3.02	-2.65	-1.64	-6.62	-4.37	-0.29	0.70