Unravelling the sensing efficacy of graphene oxide towards hazardous volatile organic compounds in polyurethane industry

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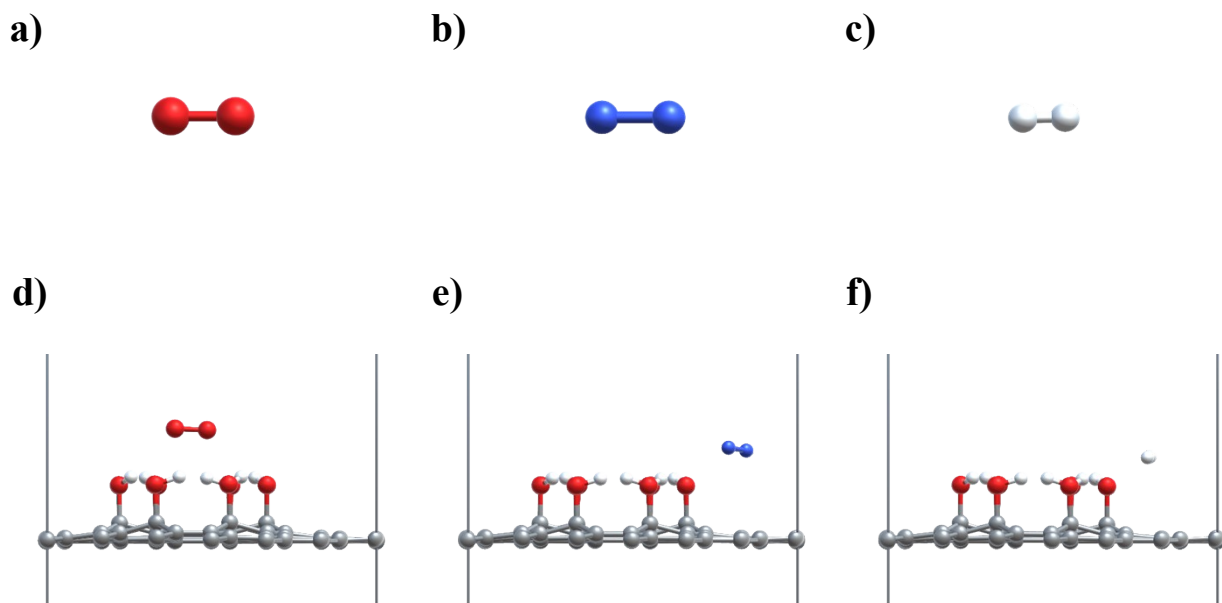
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Supporting information
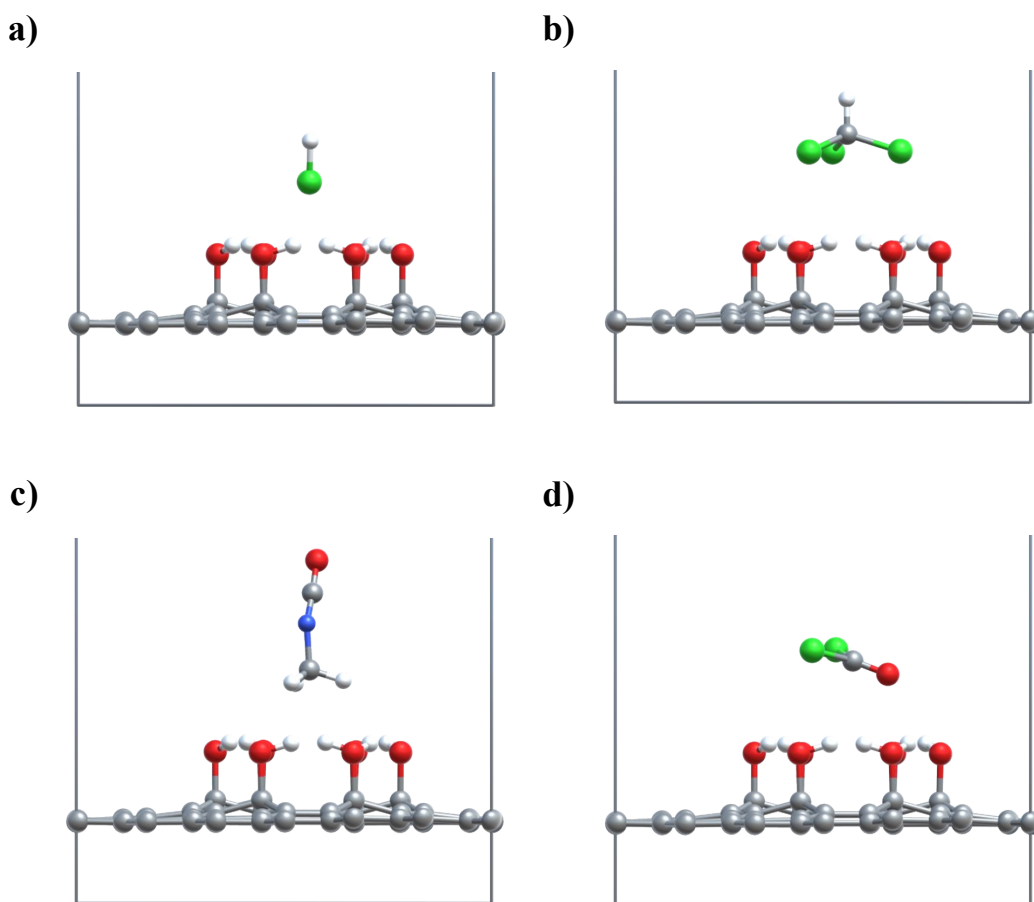
Figure S1. Geometry optimized adsorbed orientations of a) HCl, b) TCM, c) MIC, and d) PhG analytes placed above the hexahydroxyl ring system

Figure S2. Optimized structures of a) O_2, b) N_2, and c) H_2 and their most stable adsorbed conformations represented under d) GO-O_2, e) GO-N_2, and f) GO-H_2, respectively

Table S1. Computed adsorption energies (in eV) of O_2, N_2, and H_2 adsorbed onto GO slab and its corresponding shortest interaction distance (in Å)

Adsorbed slab	E_{ads}	
	VOCs placed outside hydroxyl core	VOCs placed above hydroxyl core
GO-O_2	-0.20	-0.22
GO-N_2	-0.12	-0.10
GO-H_2	-0.08	-0.06