Supplementary Material

Theoretical insights into sensing of hexavalent chromium on buckled and planar polymeric carbon nitride nanosheets of heptazine and triazine structures

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Table S1. QTAIM bond order and topological data evaluated at the bond critical points (BCPs) at the M06/Def2-TZVP level of theory.

Structure	BCP	ρ	λ_1	λ_2	λ_3	$\nabla^2\rho$	BO*
CNT1-Cr	Cr–N1	0.115	–0.157	–0.092	0.826	0.577	1.233
	Cr–N2	0.115	–0.160	–0.094	0.819	0.565	1.243
	Cr–N3	0.114	–0.159	–0.093	0.817	0.564	1.241
CNT2-Cr	Cr–N1	0.123	–0.177	–0.101	0.853	0.574	1.229
	Cr–N2	0.141	–0.251	–0.179	0.975	0.546	1.304
	Cr–N3	0.146	–0.263	–0.185	1.014	0.565	1.324
CNH1-Cr	Cr–N1	0.078	–0.132	–0.043	0.530	0.355	0.969
	Cr–N2	0.039	–0.044	–0.014	0.230	0.172	0.704
	Cr–N3	0.021	–0.015	–0.011	0.099	0.073	0.511
	Cr–N4	0.019	–0.015	–0.014	0.090	0.061	0.473
	Cr–N5	0.029	–0.025	–0.009	0.161	0.127	0.609
	Cr–N6	0.071	–0.117	–0.034	0.479	0.327	0.940
CNH2-Cr	Cr–N1	0.066	–0.104	–0.023	0.416	0.290	0.897
	Cr–N2	0.050	–0.066	–0.024	0.300	0.211	0.793
	Cr–N3	0.027	–0.027	–0.024	0.134	0.084	0.603
	Cr–N4	0.011	–0.011	–0.002	0.047	0.034	0.255
	Cr–N5	0.023	–0.020	–0.012	0.112	0.080	0.523
	Cr–N6	0.062	–0.093	–0.043	0.400	0.264	0.901

* fuzzy bond order

Table S2. Adsorption energy (kcal/mol) of Cr(VI) on different structures of graphitic carbon nitride at the M06/Def2-TZVP level of theory.

Adsorption complex	ΔE_{ads}
CNT1-Cr	–4124.71
CNT2-Cr	–3976.27
CNH1-Cr	–4271.09
CNH2-Cr	–4178.25

Table S3. Distortion energies (kcal/mol) calculated for the optimized structures of g-C_3N_4 at the M06/Def2-TZVP level of theory.

Structure	ΔE_{dist}	$\Delta E_{dist}/\Delta E_{ads}$ (%)
CNT1	20.453	0.50
CNT2	47.805	1.20
CNH1	11.464	0.27
CNH2	16.283	0.39

The distortion energy has been estimated as follows:

$$\Delta E_{dist} = E(\mathbf{1}) - E(\mathbf{2}) \quad \text{(S1)}$$

where ΔE_{dist} signifies the distortion energy, and $E(\mathbf{1})$ and $E(\mathbf{2})$ show the energies of the carbon nitride nanosheets before and after the adsorption of the chromium ion, respectively.