Supporting Information

Selective detection and removal of picric acid by C_2N surface from a mixture of nitro-explosives

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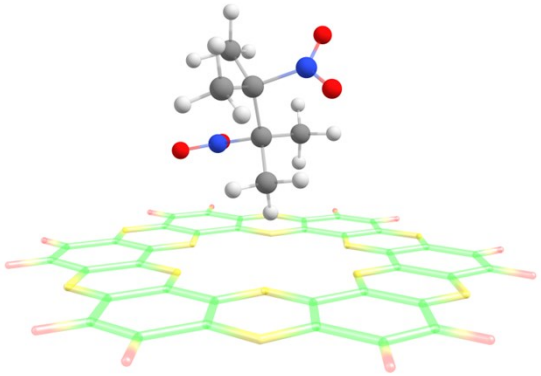

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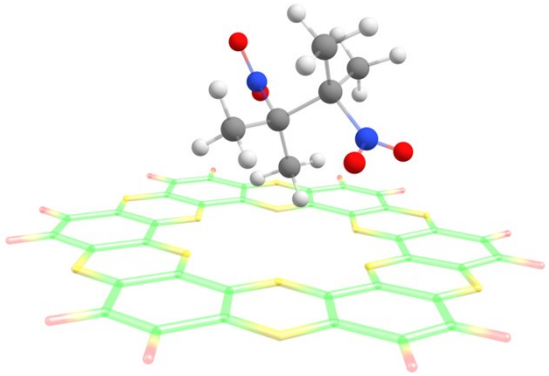

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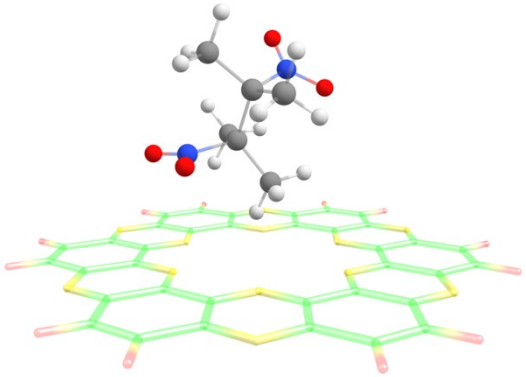

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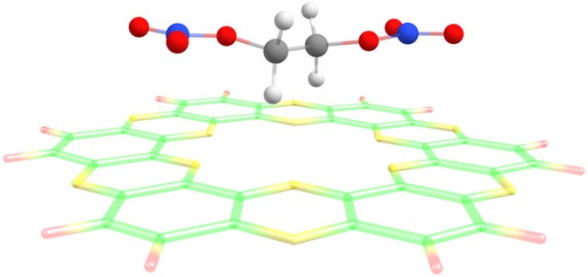

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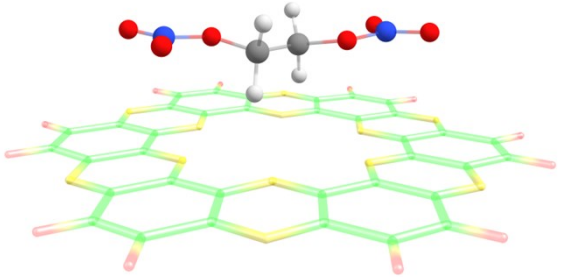

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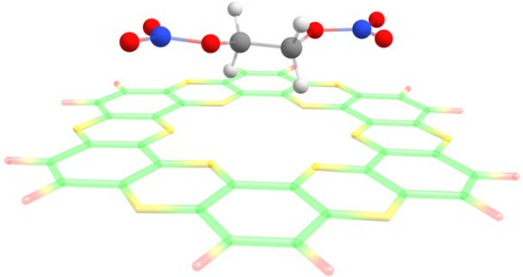

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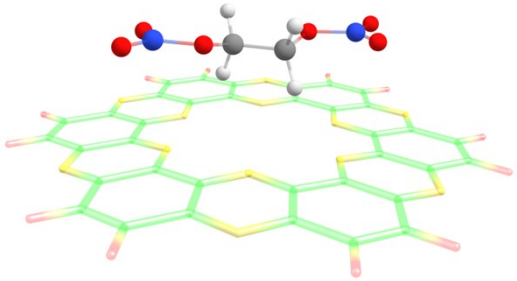

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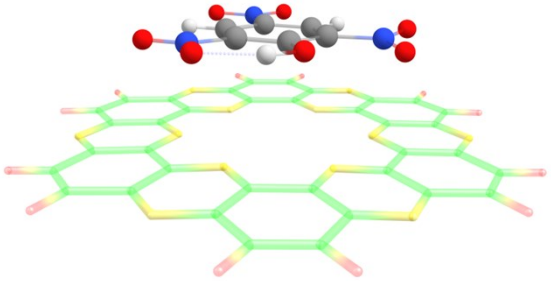

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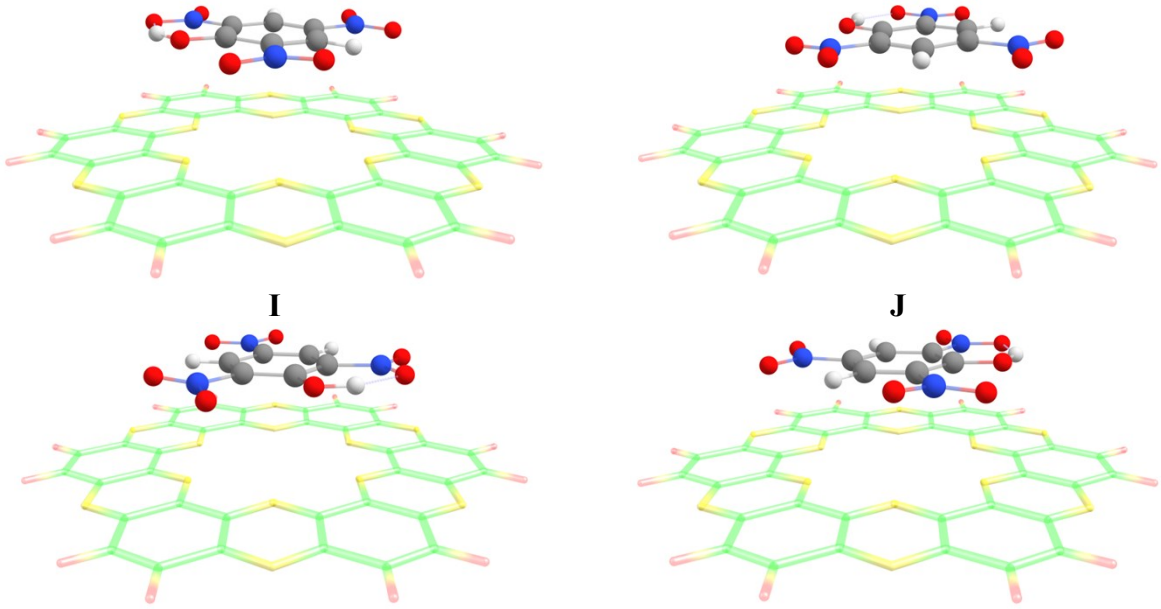
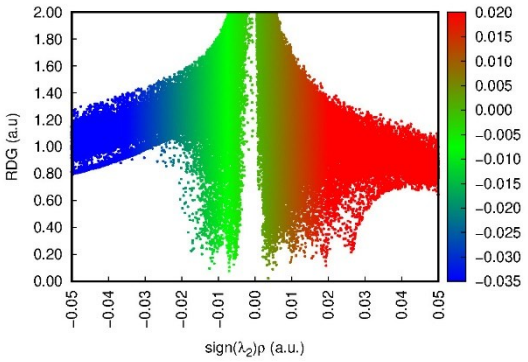
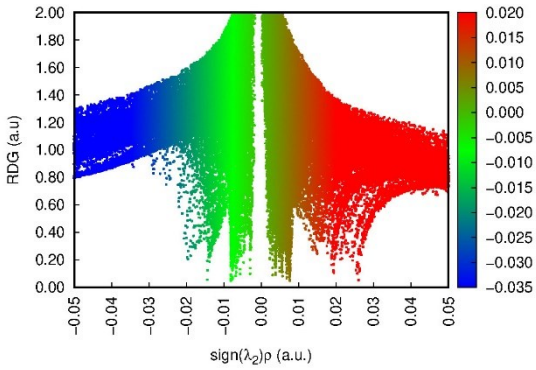


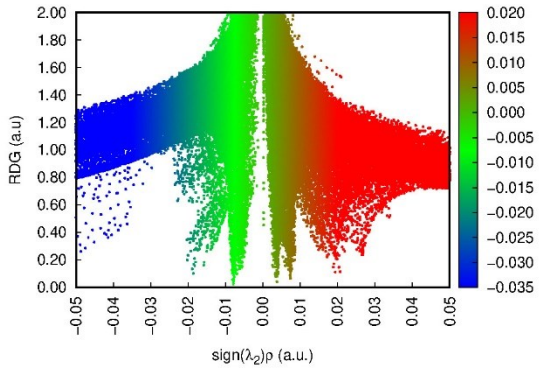
Figure S1. The least stable optimized geometries of DMNB@C_2N (A-C), EGDN@C_2N (D-G) and PA@C_2N (H-L) complexes at M05-2X/6-31++G(d,p) level of theory.



DMNB@C_2N



EGDN@C_2N



PA@C_2N

Figure S2. The 2D-NCI analysis isosurfaces of analytes@C_2N (iso value = 0.05 a.u.)

Table S1. The SAPT0 interaction energies (kcal/mol) of analytes@C_2N.

Analytes	E_{elst} (%)	E_{exch}	E_{ind} (%)	E_{disp} (%)	E_{SAPT0}
DMNB@C_2N	-12.16 (29.06)	19.40	-4.40 (10.52)	-25.29 (60.42)	-22.46
EGDN@C_2N	-19.61 (34.72)	26.15	-6.42 (11.36)	-30.45 (53.92)	-30.33
PA@C_2N	-19.41 (26.87)	32.67	-6.59 (9.13)	-46.23 (64.01)	-39.56

Table S2. The values of topological parameter of BCPs obtained from QTAIMs analysis

Analytes@C_2N	**C_2N---Analyte**	**ρ**	**$\nabla^2\rho$**	**G (r)**	**V (r)**	**H (r)**	**V(r)/G(r)**	**E_{int} (kcal/mol)**
	N1—H8	0.007	0.025	0.0051	-0.0039	0.0011	-0.775	-1.23
	N3—H9	0.006	0.02	0.0042	-0.0033	0.0009	-0.784	-1.02
	N2—H9	0.011	0.033	0.0073	-0.0065	0.0008	-0.885	-2.04
DMNB@C_2N	N3—H10	0.005	0.017	0.0036	-0.0028	0.0008	-0.790	-0.89
	N4—H11	0.005	0.018	0.0037	-0.0029	0.0008	-0.782	-0.91
	N4—H12	0.006	0.020	0.0042	-0.0032	0.0009	-0.779	-1.02
	N5—O13	0.008	0.027	0.0059	-0.0053	0.0007	-0.884	-1.65

	N5—H12	0.013	0.038	0.0087	-0.008	0.0007	-0.915	-2.49
	C6—O14	0.008	0.027	0.0059	-0.0049	0.0010	-0.836	-1.55
	N7—H8	0.007	0.025	0.005	-0.0039	0.0012	-0.770	-1.22
EDGN@C_2N	N1—H9	0.014	0.043	0.0101	-0.0094	0.0006	-0.939	-2.96
	C2—O10	0.008	0.027	0.006	-0.0051	0.0009	-0.853	-1.60
	N3—O13	0.008	0.028	0.0066	-0.0061	0.0005	-0.925	-1.90
	N3—N11	0.008	0.032	0.0067	-0.0055	0.0012	-0.820	-1.72
	C4—O12	0.007	0.024	0.0053	-0.0046	0.0007	-0.872	-1.45
	N5—H14	0.014	0.043	0.0101	-0.0094	0.0006	-0.939	-2.96
	C6—O16	0.008	0.027	0.0060	-0.0051	0.0009	-0.853	-1.60
	C6—O18	0.007	0.024	0.0053	-0.0046	0.0007	-0.872	-1.45
	N7—N17	0.008	0.032	0.0067	-0.0055	0.0012	-0.820	-1.72
	N7—O15	0.008	0.028	0.0066	-0.0061	0.0005	-0.925	-1.90

Table S3. The recovery time (s) time of sensor at different temperature (K)

Analytes@C_2N	**298K**	**350K**	**400K**
DMNB@C_2N	$2.60x10^{-04}$	$1.46\ x10^{-05}$	$1.86\ x10^{-06}$
EGDN@C_2N	$2.02\ x10^{+01}$	$2.13\ x10^{-01}$	8.17 x10-03
PA@C_2N	$3.52\ x10^{+01}$	$3.42\ x10^{-01}$	$1.24\ x10^{-02}$