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Density Functional Theory Investigation of NO_2 Gas Adsorption Properties on $X_{12}Y_{12}$ Nanocages (X= B, In and Y = As, P)

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Figure

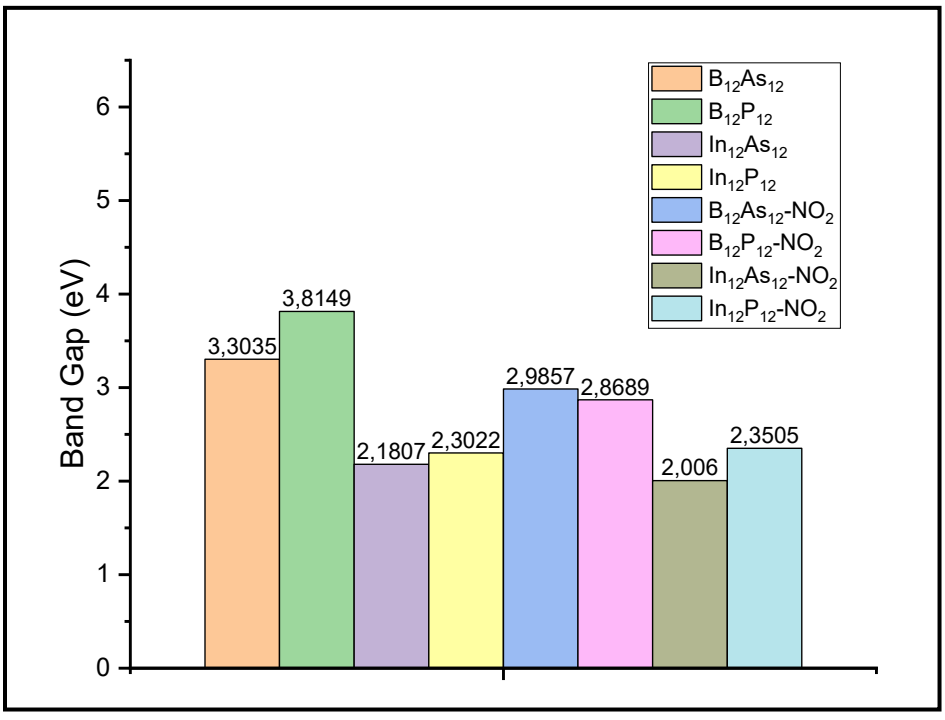


Figure S1 HOMO–LUMO energy gap across all systems

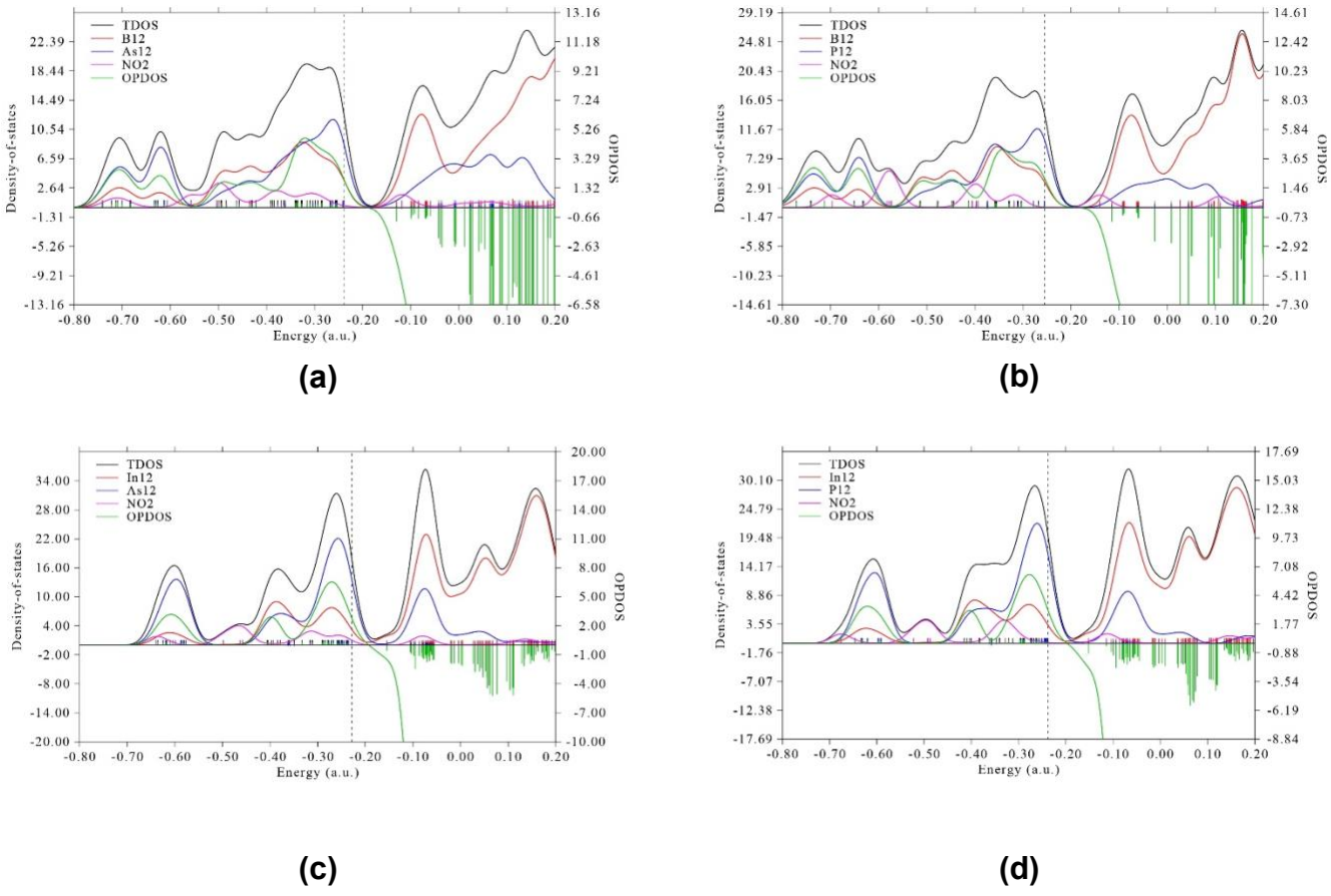
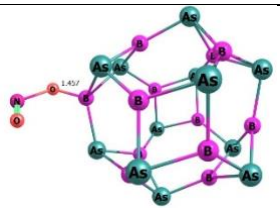
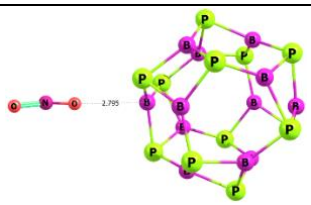
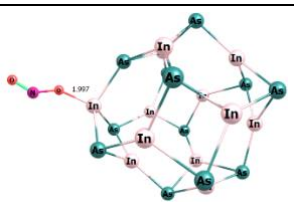
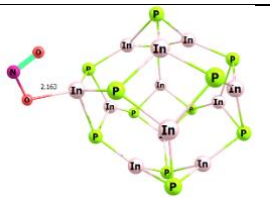
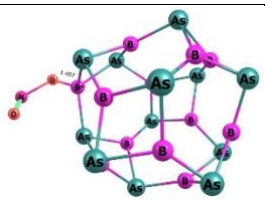
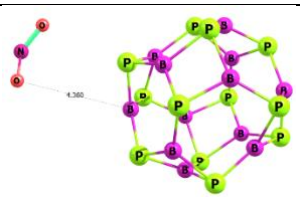
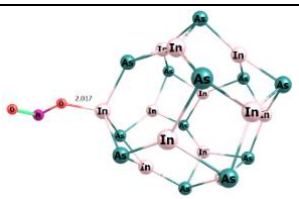
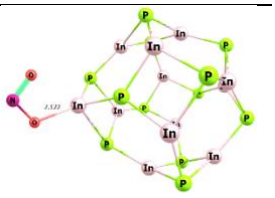


Figure S2 (TDOS), (PDOS), and (OPDOS) for NO_2 Adsorption on : (a) $B_{12}As_{12}$, (b) $B_{12}P_{12}$, (c) $In_{12}As_{12}$, and (d) $In_{12}P_{12}$

	$B_{12}As_{12}$	$B_{12}P_{12}$	$In_{12}As_{12}$	$In_{12}P_{12}$
0 fs				
500 fs				

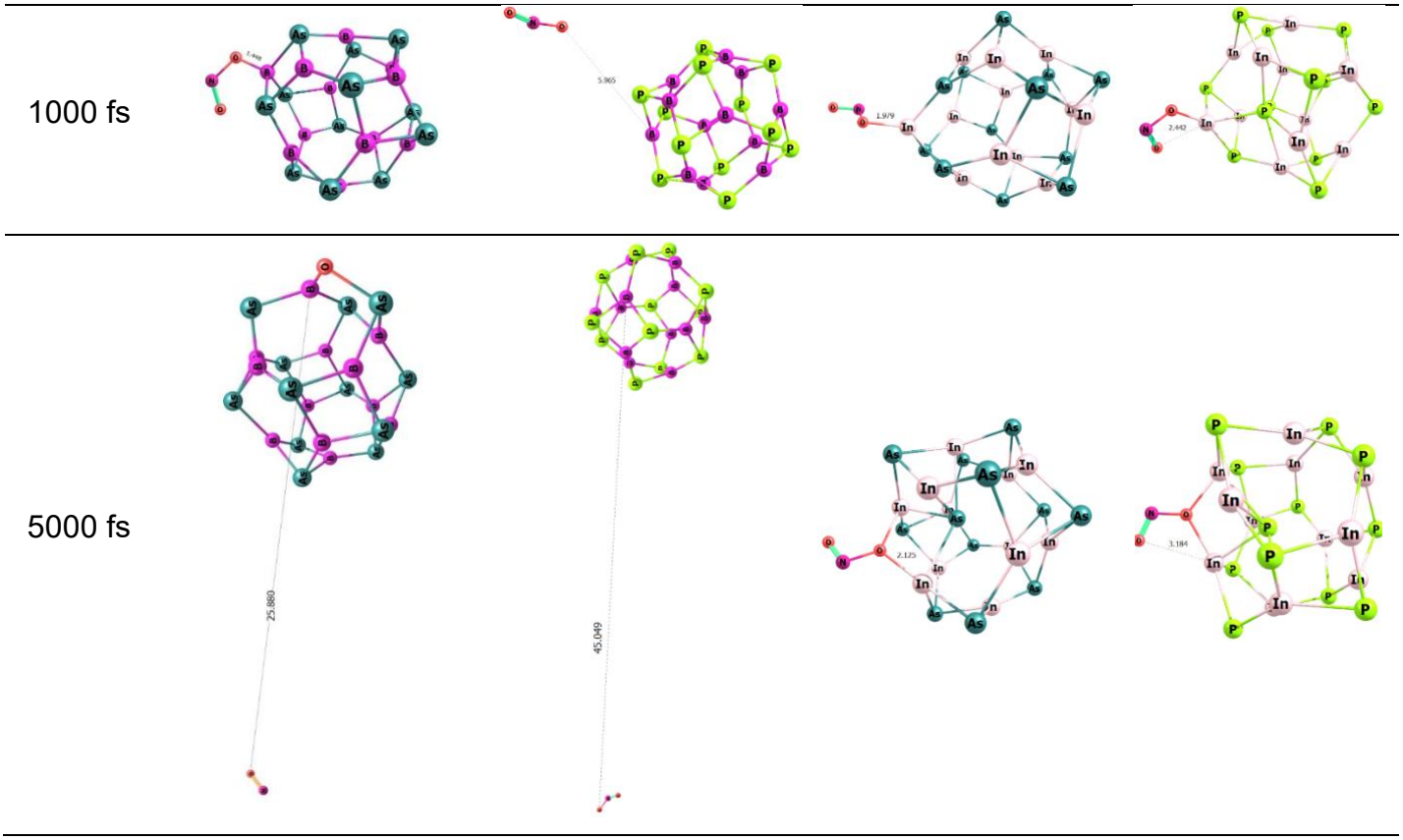


Figure S3 AIMD simulation snapshot of NO_2 Adsorption on $B_{12}As_{12}$, $B_{12}P_{12}$, $In_{12}As_{12}$, $In_{12}P_{12}$

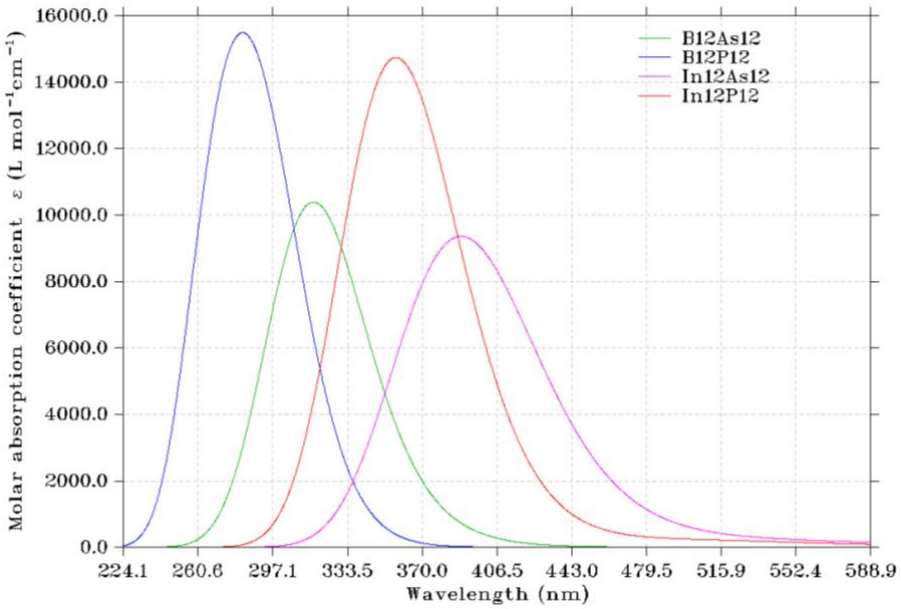


Figure S4 Uv-Vis Spectrum of $B_{12}As_{12}$, $B_{12}P_{12}$, $In_{12}As_{12}$, $In_{12}P_{12}$

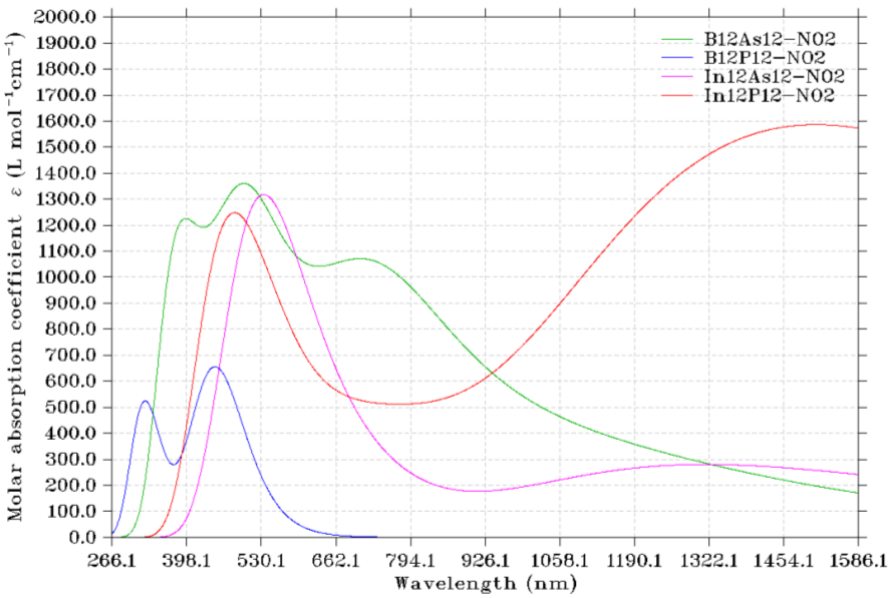


Figure S5 UV-Vis Spectrum of $B_{12}As_{12}$-NO_2, $B_{12}P_{12}$-NO_2, $In_{12}As_{12}$-NO_2, $In_{12}P_{12}$-NO_2

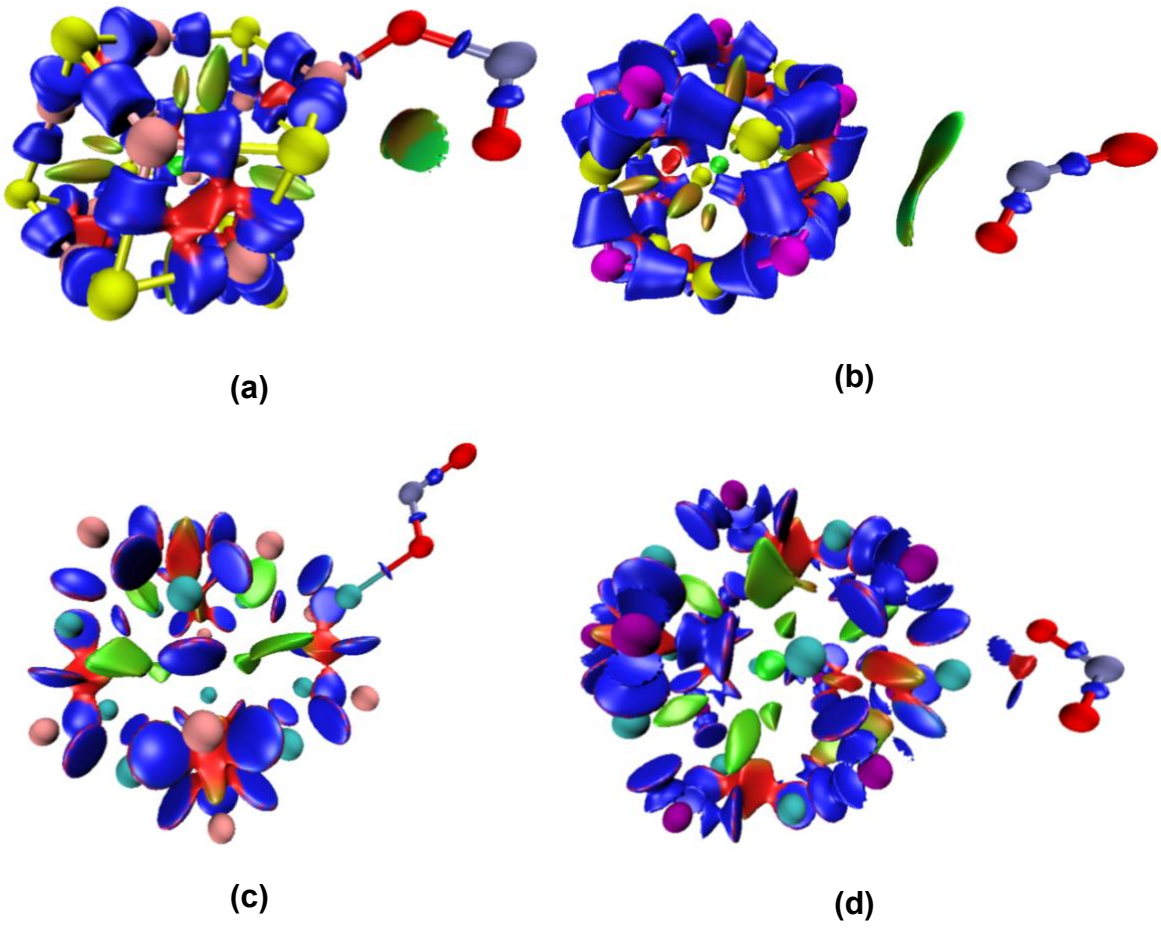
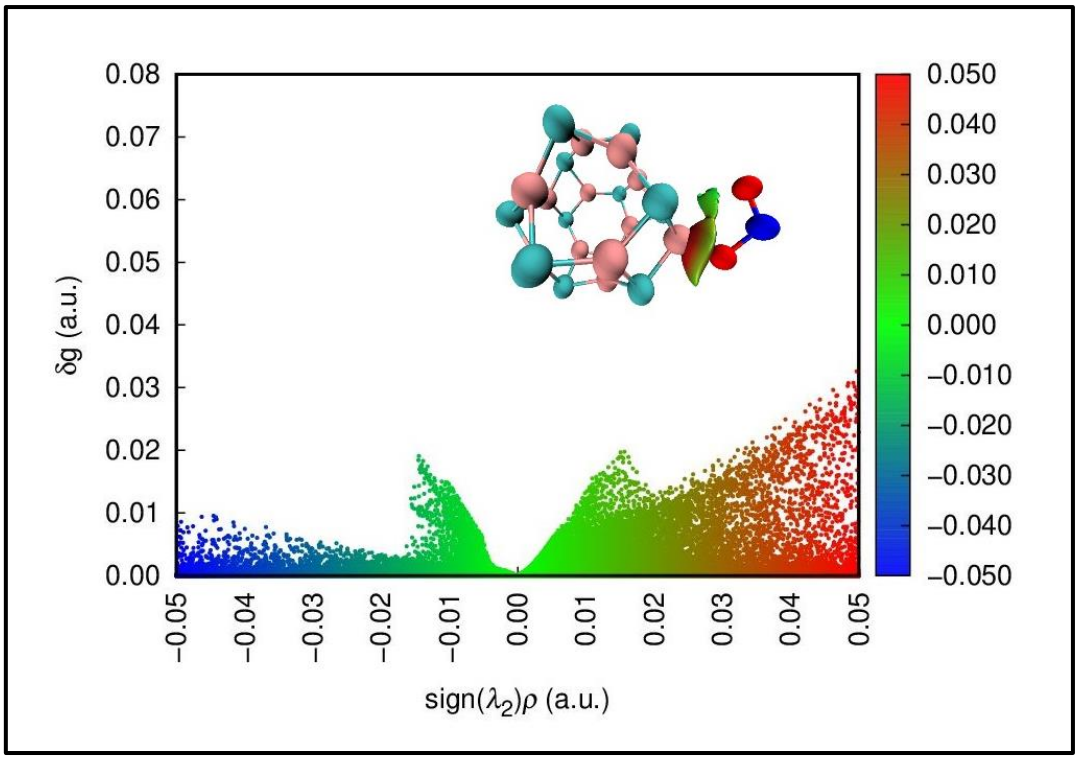
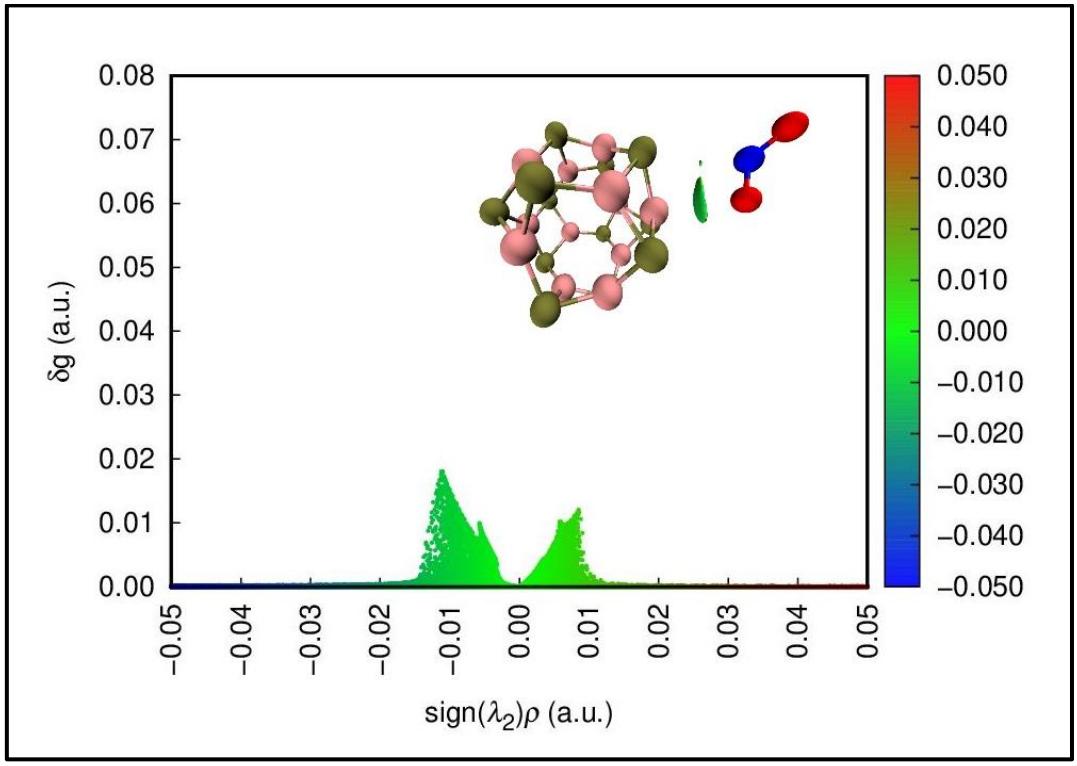


Figure S6 IRI Analysis of nanocage-gas systems: (a) $B_{12}As_{12} - NO_2$, (b) $B_{12}P_{12} - NO_2$ (c) $In_{12}As_{12} - NO_2$, and (d) $In_{12}P_{12} - NO_2$


0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0.00
δg (a.u.)
−0.05
−0.04
−0.03
−0.02
−0.01
0.00
0.01
0.02
0.03
0.04
0.05
sign(λ2)ρ (a.u.)
0.050
0.040
0.030
0.020
0.010
0.000
−0.010
−0.020
−0.030
−0.040
−0.050

(a)


0.08
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δg (a.u.)
−0.05
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−0.02
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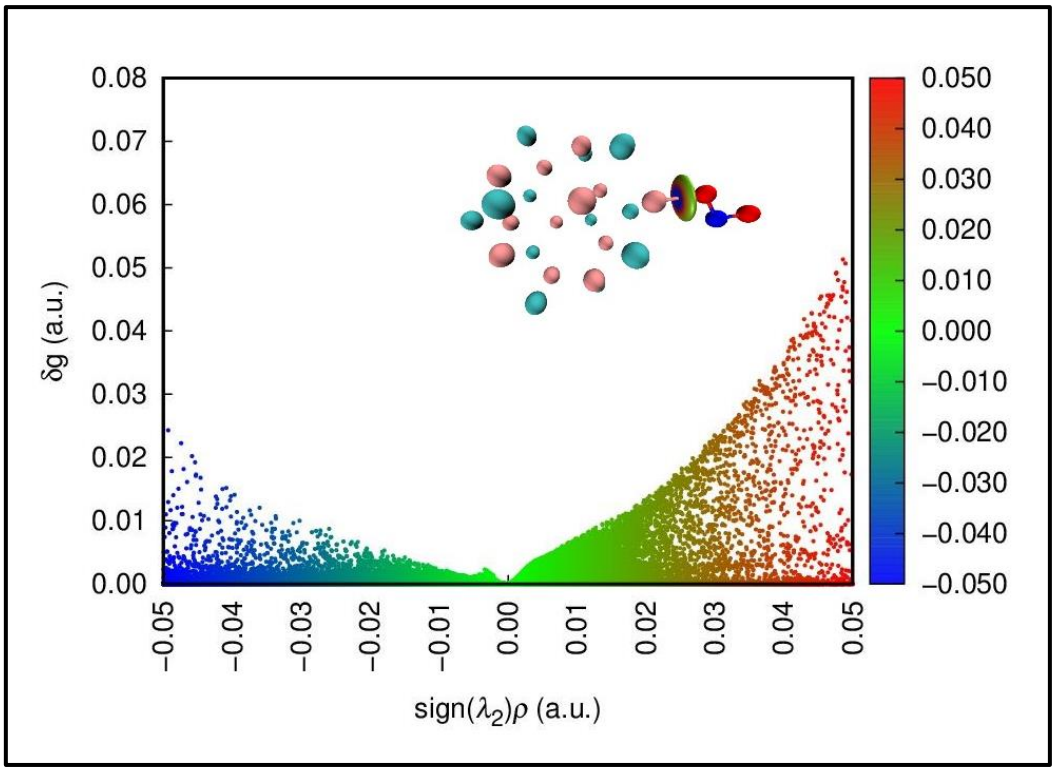
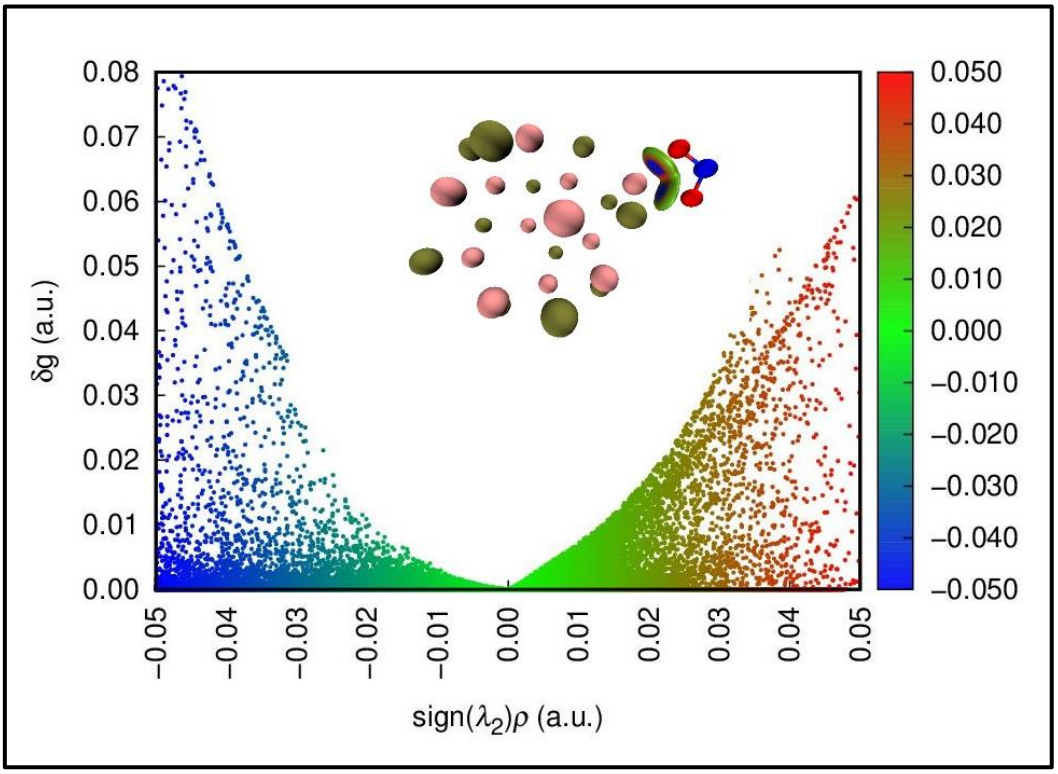
0.04
0.05
sign(λ2)ρ (a.u.)
0.050
0.040
0.030
0.020
0.010
0.000
−0.010
−0.020
−0.030
−0.040
−0.050

(b)



(c)



(d)

Figure S7 IGMH Analysis of (a) $B_{12}As_{12} - NO_2$, (b) $B_{12}P_{12} - NO_2$ (c) $In_{12}As_{12} - NO_2$, and (d) $In_{12}P_{12} - NO_2$

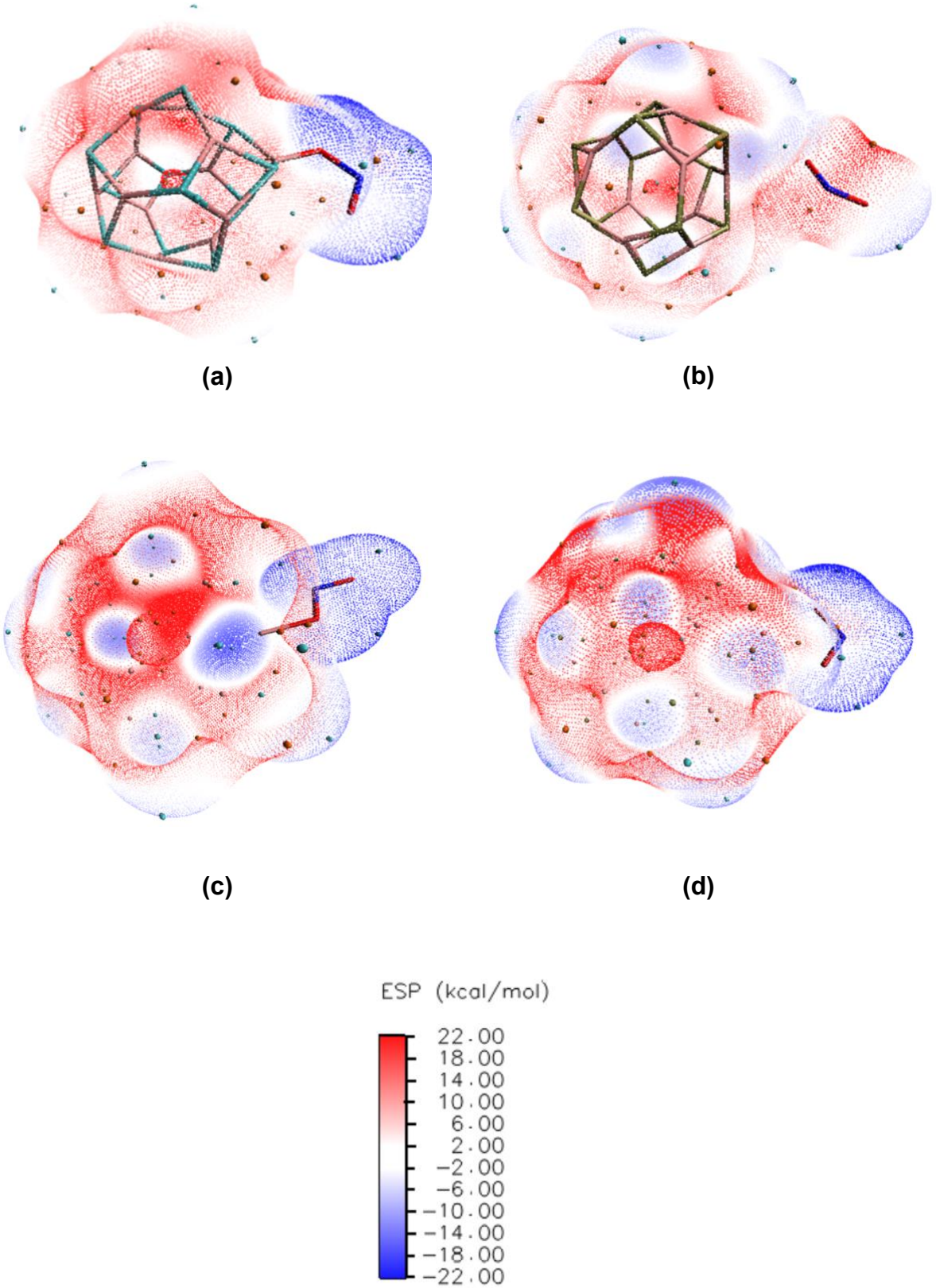


Figure S8 ESP Analysis of (a) $B_{12}As_{12} - NO_2$, (b) $B_{12}P_{12} - NO_2$ (c) $In_{12}As_{12} - NO_2$, and (d) $In_{12}P_{12} - NO_2$

Table

Table S1 Frontier Molecular Orbital Analysis: E_{HOMO}, E_{LUMO}, E_g, (IP), (EA), (μ), (η), and (S)

	E_{HOMO} (eV)	E_{LUMO} (eV)	E_g (eV)	IP (eV)	EA (eV)	μ (eV)	η (eV)	S (eV)
$B_{12}As_{12}$	-6.6921	-3.3886	3.3035	6.6921	3.3886	-5.0403	4.9978	0.1000
$B_{12}As_{12}$-NO_2	-6.5179	-3.5322	2.9857	6.5179	3.5322	-5.0250	4.7518	0.1052
$B_{12}P_{12}$	-6.9784	-3.1635	3.8149	6.9784	3.1635	-5.0709	5.3966	0.0926
$B_{12}P_{12}$-NO_2	-6.9500	-4.0811	2.8689	6.9500	4.0811	-5.5155	4.9094	0.1018
$In_{12}As_{12}$	-6.2350	-4.0543	2.1807	6.2350	4.0543	-5.1446	4.2078	0.1188
$In_{12}As_{12}$-NO_2	-6.1722	-4.1662	2.006	6.1722	4.1662	-5.1692	4.0891	0.1222
$In_{12}P_{12}$	-6.3746	-4.0724	2.3022	6.3746	4.0724	-5.2235	4.3384	0.1152
$In_{12}P_{12}$-NO_2	-6.4771	-4.1266	2.3505	6.4771	4.1266	-5.3018	4.4138	0.1133

Table S2 QTAIM Analysis of NO_2 Adsorption on $X_{12}Y_{12}$ nanocage

	ρ	$(\nabla^2\rho)$	G_{BCP}	H_{BCP}	V_{BCP}	|V/G|
$B_{12}As_{12}$-NO_2	0.151	0.5369	0.2482	-0.1141	-0.3623	-1.4597
$B_{12}P_{12}$-NO_2	0.0118	-0.1767	0.236	-0.6918	-0.9278	-3.9314
$In_{12}As_{12}$-NO_2	0.1069	0.5057	0.5135	-0.1889	-0.7025	-1.3681
$In_{12}P_{12}$-NO_2	0.7449	0.3251	0.3143	-0.9747	-0.4118	-1.3102

Table S3 NBO Analysis of NO_2 Adsorption on $X_{12}Y_{12}$ nanocage

	Donor (d)	Acceptor	E^2 (kcal/mol)	$E_{(j)}$-$E_{(i)}$ (a.u)	$F_{(i,j)}$ (a.u)
$B_{12}As_{12}$-NO_2	BD (1) N25 - O26	RY (1) B1	0.91	1.47	0.046
$B_{12}P_{12}$-NO_2	LP (1) O27	LV (1) B1	7.45	0.63	0.087
$In_{12}As_{12}$-NO_2	BD (2) N25 - O26	BD* (1) In1 - O27	0.85	1.02	0.032
$In_{12}P_{12}$-NO_2	LP (2) O27	LV (1) In1	13.24	0.52	0.105

Table S4 Charge Transfer (Q_{CT}) values from Mulliken Charge and NBO charge

	Q_{CT}	
	Mulliken	NBO
$B_{12}As_{12}$-NO_2	-0.3980	-0.0383
$B_{12}P_{12}$-NO_2	-0.4137	-0.0571
$In_{12}As_{12}$-NO_2	0.7095	1.2873
$In_{12}P_{12}$-NO_2	0.7832	1.3644

Table S5 UV-Vis Analysis

System	λ_{max}	f_o	ΔE	Domminant transition
	(nm)		(eV)	
$B_{12}As_{12}$	319.2	0.0647	3.885	HOMO-4 → HUMO
$B_{12}As_{12}$-NO_2	736	0.0171	1.685	HOMO-2 → HOMO
$B_{12}P_{12}$	292.5	0.7388	4.238	HOMO-2 → HUMO
$B_{12}P_{12}$-NO_2	450.5	0.0088	2.752	HOMO-3 → HOMO
$In_{12}As_{12}$	389	0.0771	3.187	HOMO-13 → HOMO
$In_{12}As_{12}$-NO_2	526.8	0.0053	2.353	HOMO-5 → HOMO
$In_{12}P_{12}$	357	0.1215	3.473	HOMO-16 → HOMO
$In_{12}P_{12}$-NO_2	1546.1	0.0375	0.802	HOMO-1 → HOMO