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Modeling of Magnesium decorated graphene quantum dot nanostructured for trapping AsH_3, PH_3 and NH_3 gases

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TABLE S1. Thermodynamic parameters of the optimized structures including the Enthalpy and Gibbs free energy in Benzene phase

PARMETERS	$C_{24}H_{12}$-Mg_benz	AsH_3_benz	AsH_3@$C_{24}H_{12}$-Mg_benz	NH_3_benz	NH_3@$C_{24}H_{12}$-Mg_benz	PH_3_benz	PH_3@$C_{24}H_{12}$-Mg_benz
ε_0	-1121.876	-2235.823	-3359.575	-56.567	-1178.449	-343.151	-1465.034
ε_{ZPE}	0.283	0.020	0.306	0.035	0.319	0.024	0.308
E_{tot}	0.299	0.023	0.327	0.037	0.339	0.027	0.329
H_{corr}	0.300	0.024	0.328	0.038	0.340	0.028	0.330
G_{corr}	0.237	-0.000	0.252	0.016	0.266	0.003	0.255
$\varepsilon_0 + \varepsilon_{ZPE}$	-1121.593	-2235.803	-3359.268	-56.532	-1178.130	-343.127	-1465.726
$\varepsilon_0 + E_{tot}$	-1121.577	-2235.800	-3359.247	-56.529	-1178.110	-343.124	-1465.705
$\varepsilon_0 + H_{corr}$	-1121.576	-2235.799	-3359.246	-56.528	-1178.109	-343.123	-1465.704
$\varepsilon_0 + G_{corr}$	-1121.639	-2235.823	-3359.323	-56.551	-1178.183	-343.148	-1465.779
$\Delta_f H^*$(298K)			-1.871		-0.005		-1.005
$\Delta_f G^*$ (298)			-1.861		0.007		-0.992

PARMETERS	$C_{24}H_{12}$-Mg_EtOH	AsH_3_EtOH	$AsH_3@C_{24}H_{12}$-Mg_EtOH	NH_3_EtOH	$NH_3@C_{24}H_{12}$-Mg_EtOH	PH_3_EtOH	$PH_3@C_{24}H_{12}$-Mg_EtOH
ε_0	-1121.885	-2235.827	-3359.584	-56.569	-1178.460	-343.151	-1465.044
ε_{ZPE}	0.283	0.020	0.306	0.035	0.318	0.024	0.309
E_{tot}	0.299	0.023	0.327	0.037	0.338	0.027	0.329
H_{corr}	0.300	0.024	0.328	0.038	0.339	0.028	0.330
G_{corr}	0.237	-0.000	0.252	0.016	0.265	0.003	0.255
$\varepsilon_0 + \varepsilon_{ZPE}$	-1121.603	-2235.806	-3359.278	-56.535	-1178.142	-343.127	-1464.735
$\varepsilon_0 + E_{tot}$	-1121.586	-2235.804	-3359.257	-56.532	-1178.122	-343.124	-1464.714
$\varepsilon_0 + H_{corr}$	-1121.585	-2235.803	-3359.256	-56.531	-1178.121	-343.123	-1464.714
$\varepsilon_0 + G_{corr}$	-1121.649	-2235.827	-3359.332	-56.554	-1178.195	-343.148	-1464.789
$\Delta_f H^*(298K)$			-1.876		-0.005		-0.006
$\Delta_f G^*(298)$			1.856		-0.015		0.008

TABLE S2. Thermodynamic parameters of the optimized structures including the Enthalpy and Gibbs free energy in Ethanol phase

PARMETERS	$C_{24}H_{12}$-Mg_H_2O	AsH_3_H_2O	AsH_3@$C_{24}H_{12}$-Mg_H_2O	NH_3_H_2O	NH_3@$C_{24}H_{12}$-Mg_H_2O	PH_3_H_2O	PH_3@$C_{24}H_{12}$-Mg_H_2O
ε_0	-1121.886	-2235.825	-3359.585	-56.570	-1178.461	-343.151	-1465.045
ε_{ZPE}	0.283	0.020	0.306	0.035	0.319	0.024	0.309
E_{tot}	0.299	0.023	0.327	0.037	0.339	0.027	0.329
H_{corr}	0.300	0.024	0.328	0.038	0.340	0.028	0.330
G_{corr}	0.236	-0.000	0.252	0.016	0.265	0.003	0.255
$\varepsilon_0 + \varepsilon_{ZPE}$	-1121.603	-2235.805	-3359.279	-56.535	-1178.143	-343.127	-1465.736
$\varepsilon_0 + E_{tot}$	-1121.587	-2235.802	-3359.258	-56.532	-1178.122	-343.124	-1465.715
$\varepsilon_0 + H_{corr}$	-1121.586	-2235.801	-3359.257	-56.531	-1178.121	-343.123	-1465.714
$\varepsilon_0 + G_{corr}$	-1121.650	-2235.826	-3359.333	-56.554	-1178.196	-343.148	-1465.790
$\Delta_f H^*(298K)$			-1.870		-0.004		-1.005
$\Delta_f G^*(298)$			-1.857		0.008		-0.992

TABLE S3. Thermodynamic parameters of the optimized structures including the Enthalpy and Gibbs free energy in Water phase.