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Supporting Information for

Ammonia Sensor Design from Interaction with Metallo-Phthalocyanines: DFT Analysis of Rovibrational and Thermodynamics Parameters

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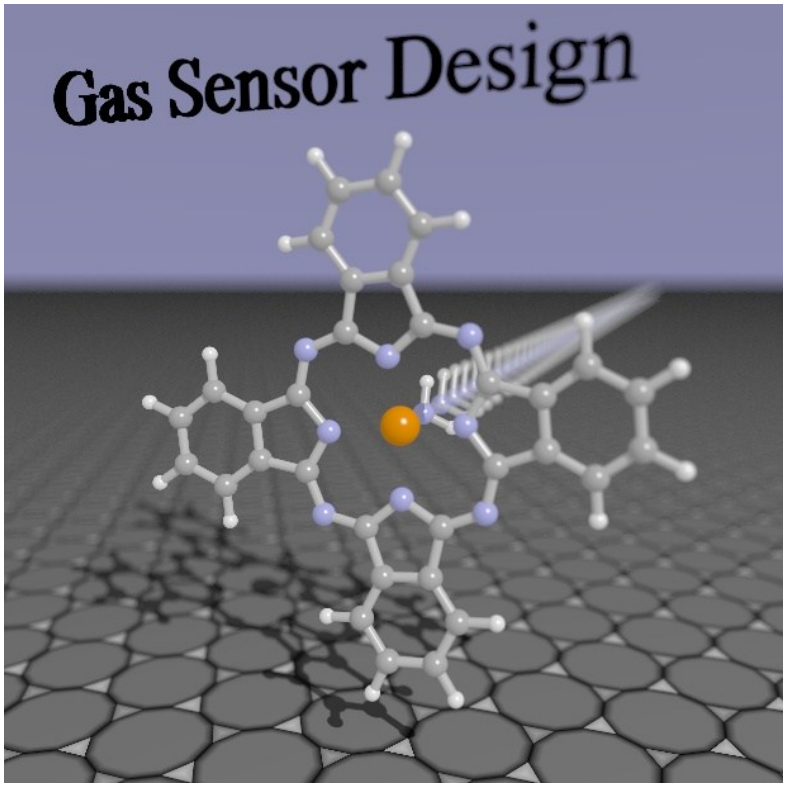

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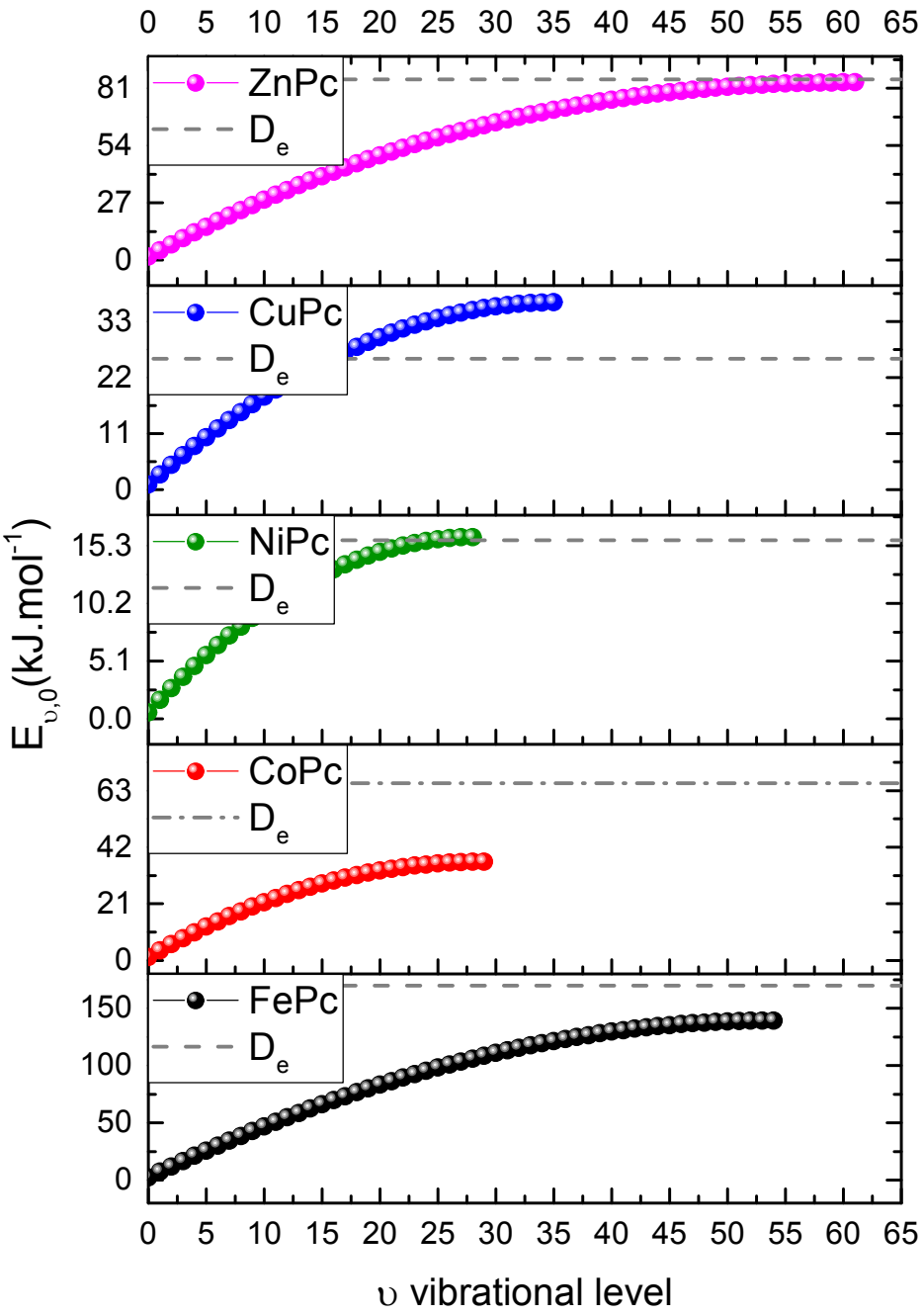

Figure S1. Maximum vibrational number (υ_{max}) obtained from the B3LYP/6-311G(d)/LANL2DZ BECs according to protocol C. D_e was obtained from the difference between the geometry in equilibrium and in the asymptotic region.

Table S1. Fitted Rydberg of sixth degree parameters for MPc-NH3 BECs obtained from B3LYP/6-311G(d)/LANL2DZ without corrections.

System	c_1	c_2	c_3	c_4	c_5	c_6	R_e (bohr)	D_e (hartree)	χ^2 (10^{-9}) (hartree)
FePc	1.015707	-0.290585	0.103751	-0.019521	0.006461	-0.000522	3.78	0.060010	8.2
CoPc	1.17530	-0.04033	0.09761	0.00379	0.00788	0.00001	4.29	0.02201	0.81
NiPc	0.776410	-0.072623	0.175097	-0.023183	0.000610	0.000000	5.34	0.004790	0.092
CuPc	0.529297	-0.560815	0.256448	-0.048415	0.003958	-0.000119	4.62	0.012187	27
ZnPc	0.755789	-0.445929	0.261737	-0.069954	0.009232	-0.000465	4.18	0.030980	190

Table S2. Fitted Rydberg of sixth degree parameters for MPc-NH3 BECs obtained from B3LYP/6-311G(d)/LANL2DZ including BSSE corrections.

System	c_1	c_2	c_3	c_4	c_5	c_6	R_e (bohr)	D_e (hartree)	χ^2 (10^{-9}) (hartree)
FePc	1.361873	0.029271	0.044745	0.007133	0.006071	-0.000244	3.79	0.05256	0.39
CoPc	1.12809	-0.25914	0.12665	-0.01226	0.00375	-0.00033	4.3	0.0153	6.7
NiPc	0.624951	0.023064	-0.016486	-0.079889	0.03167	-0.003339	6.61	0.000396	1,7
CuPc	1.200324	-0.070811	0.097429	-0.000222	0.008476	-0.001711	4.76	0.00675	1.7
ZnPc	1.165452	-0.064404	0.073175	-0.020727	0.008914	-0.001828	4.28	0,.2339	1.2

Table S3. Fitted Rydberg of sixth degree parameters for MPc-NH3 BECs obtained from B3LYP/6-311G(d)/LANL2DZ including BSSE and dispersion corrections.

System	c_1	c_2	c_3	c_4	c_5	c_6	R_e (bohr)	D_e (hartree)	χ^2 (10^{-9}) (hartree)
FePc	1.26311	0.00290	0.07000	0.00303	0.00351	9.64375E-6	3.76	0.06462	0.71
CoPc	1.32582	0.15889	0.11552	0.01156	0.00204	6.25266E-4	4.24	0.02502	0.43
NiPc	2.10717	1.75478	0.71708	0.18422	0.13353	0.05605	5.40	0.00601	2.12
CuPc	1.92256	0.94297	0.20126	-0.07478	-0.03359	0.01693	4.59	0.00979	1.19
ZnPc	1.24593	0.15897	0.10305	-0.00579	0.00555	1.74872E-5	4.23	0.03239	0.18

Table S4. Thermodynamic quantites for the MPc-NH_3 interaction calculated from rovibrational constants obtaind utilizing BSSE and GD3BJ corrections (Protocol C).

T = 298K	FePc	CoPc	NiPc	CuPc	ZnPc
$\Delta G\ (kJ.mol^{-1})$	-150.06	-48.76	-3.39	-9.84	-67.52
$\Delta H\ (kJ.mol^{-1})$	-172.61	-69.04	-18.49	-29.10	-88.41
$\Delta S\ (J.mol^{-1})$	-75.627	-68.02	-50.65	-64.61	-70.08

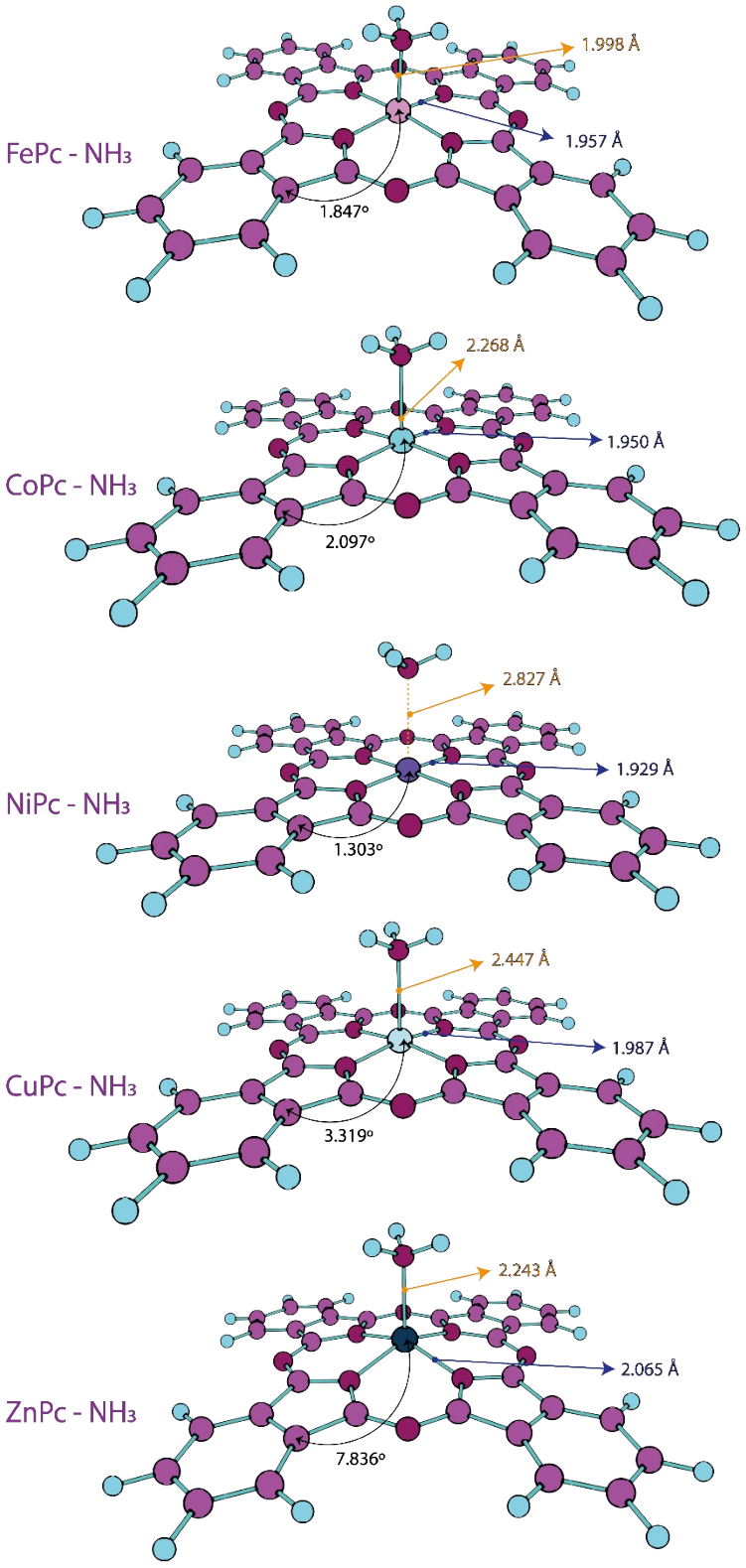

Figure S2. Optimized geometries for MPc-NH_3 interaction obtained via B3LYP/6-311G(d)/LANL2DZ level of theory (protocol C).

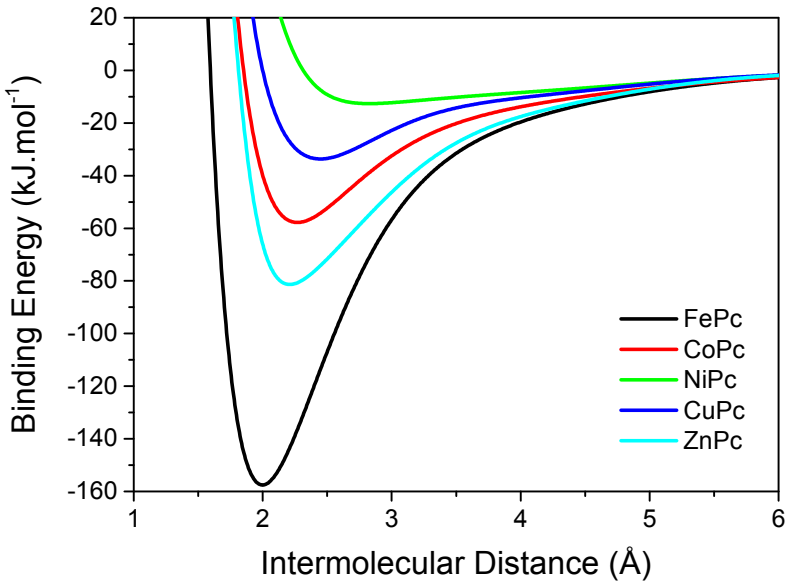

Figure S3. BECs for the MPc-NH_3 interaction without corrections (protocol A).

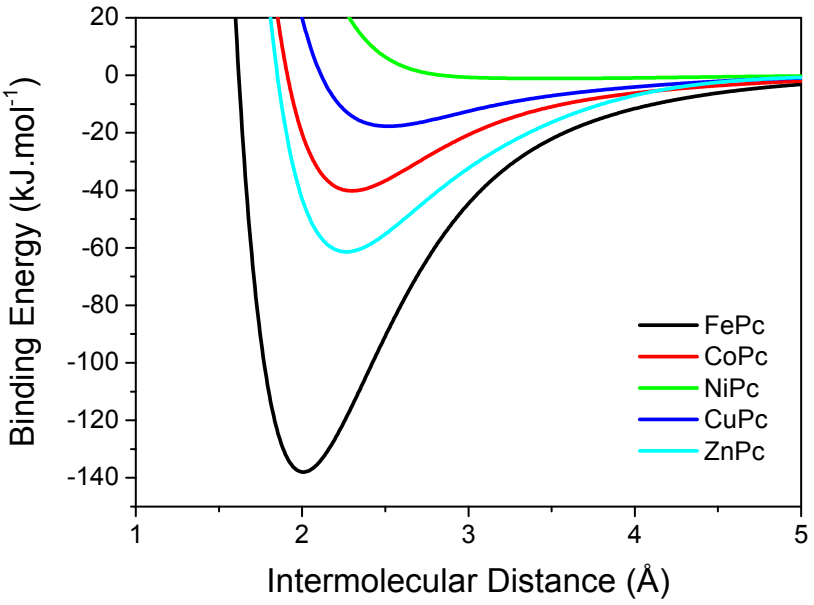

Figure S4. BECs for the MPc-NH_3 interaction with BSSE corrections (protocol B).

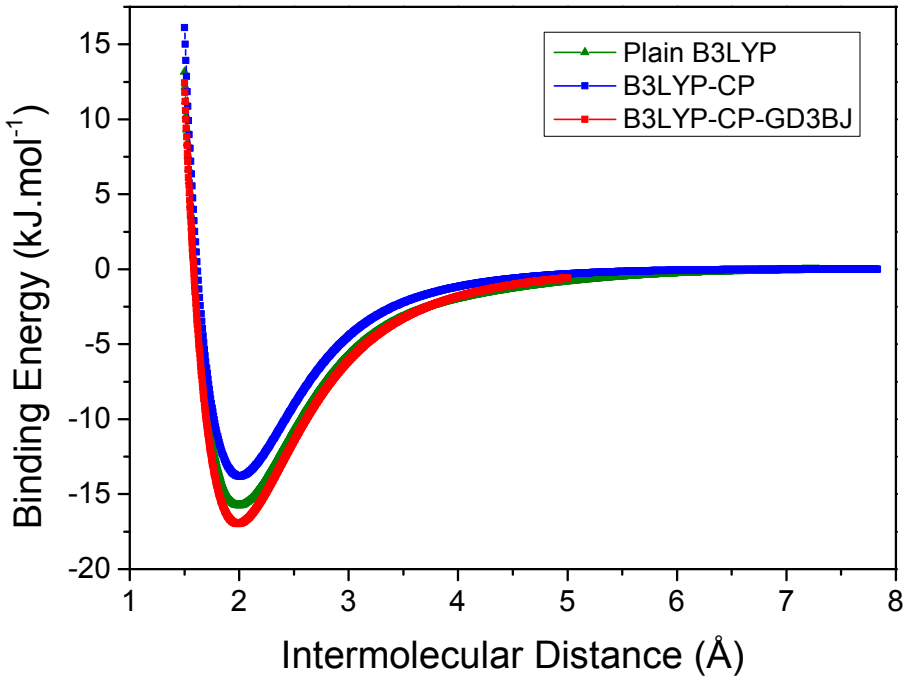

Figure S5. FePc-NH_3 BECs for plain B3LYP/6-311G(d)/LANL2DZ calculation (green), including only BSSE corrections (blue) and including both of BSSE and Dispersive corrections (red).

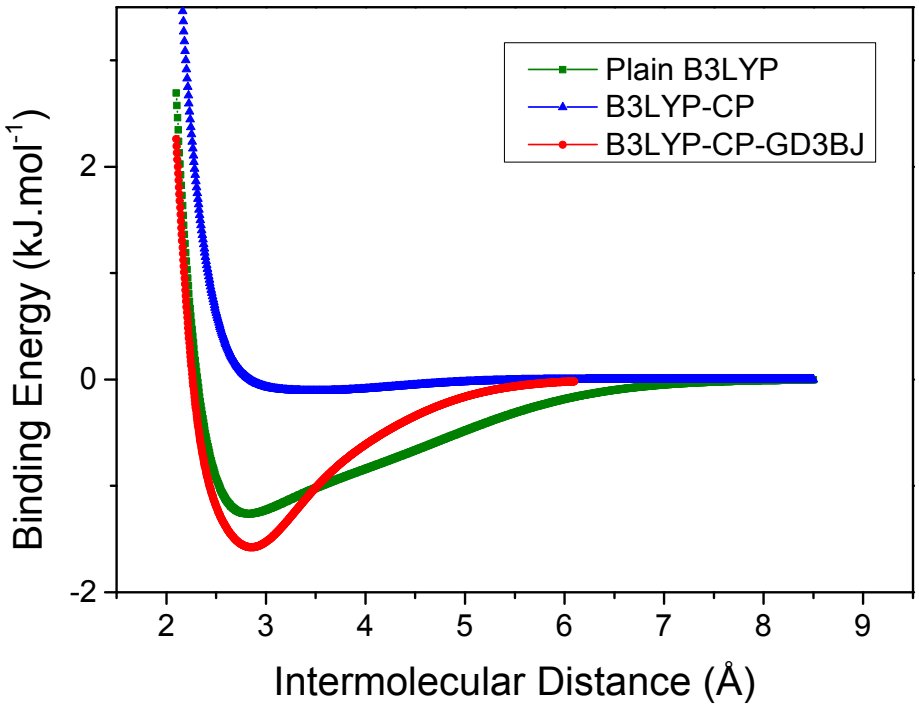

Figure S6. NiPc-NH_3 BECs for plain B3LYP/6-311G(d)/LANL2DZ calculation (green), including only BSSE corrections (blue) and including both of BSSE and dispersive corrections (red).