Aqueous solvation of $Hg(OH)_2$. Energetic and dynamical density functional theory studies of the $Hg(OH)_2$ –$(H_2O)_n$ (*n*=1-24) structures.

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Supplementary material

Table S1. Calculated NPA charges of Hg, O, H and O (directly linked to Hg) atoms in gaseous and solvated $Hg(OH)_2$ systems.

Water Molecules	**Hg**	**O(H)**	**O(H)**	**O1 (H_2O)**	**O2 (H_2O)**	**O3 (H_2O)**
0	0.98	-0.98	-0.98	--	--	--
1	1.12	-1.07	-1.03	-1.00	--	--
2	1.14	-1.09	-1.03	-1.03	--	--
3	1.16	-1.07	-1.07	-1.06	--	--
4	1.16	-1.08	-1.07	-1.03	-1.04	--
5	1.19	-1.08	-1.07	-1.03	-1.02	--
6	1.18	-1.08	-1.09	-1.05	-1.01	--
7	0.98	-1.04	-1.04	-1.00	-1.01	
8	0.98	-1.08	-1.04	-1.02	-1.01	-1.01
12	1.20	-1.12	-1.12	-1.07	-1.04	-1.03
15	1.17	-1.15	-1.13	-1.08	-1.03	-1.02
16	1.00	-1.14	-1.13	-1.05	-1.03	-1.04
24	1.03	-1.13	-1.10	-1.04	-1.05	-1.06

Table S2. Optimized atomic coordinates (at 0 K) of the final solvated cluster $Hg(OH)_2$-$(H_2O)_{24}$

	Coordinates (Angstroms)		
	X	Y	Z
O	-1.770470	-1.492280	-3.276406
O	-1.073834	-1.911928	-0.696651
Hg	0.334829	-0.458191	-0.397339
O	-0.466515	0.264520	2.192626
O	-3.562183	-1.491148	-0.059395
O	1.725536	1.084790	-0.151591

O	-1.423220	-1.783482	3.487476
O	-4.415446	-0.714302	-2.451491
O	2.347330	1.768773	-2.630974
O	-2.025867	2.285769	1.480315
O	-0.656208	4.544854	1.865661
O	-4.338565	0.741265	1.331691
O	4.242603	-0.155293	-2.312338
O	2.134395	0.894202	2.629353
O	3.931980	2.867650	2.082801
O	-0.351710	0.823102	-2.732556
O	2.767355	-1.697550	1.778461
O	2.595568	-2.021272	-0.923599
O	-0.164698	-4.288667	0.300477
O	0.684489	-3.407438	2.566225
O	1.675839	3.790660	0.503699
O	-4.150494	-1.681461	2.651525
O	2.016339	-4.673917	-1.341042
O	4.420585	0.492320	0.353444
O	-0.616489	4.945452	-0.918983
O	-1.830917	2.529261	-1.246477
O	-4.445584	1.933399	-1.448808
H	-2.698475	-1.219053	-3.184578
H	-1.276225	-0.657303	-3.351799
H	-0.892497	1.518099	-2.288273

H	0.478002	1.235796	-3.014997
H	-1.535171	3.468418	-1.272804
H	-2.800356	2.460793	-1.431676
H	-4.719621	1.728808	-0.542509
H	-4.515468	1.083030	-1.920465
H	-0.879499	5.166021	-0.011421
H	0.306942	4.680461	-0.782657
H	-4.255852	-1.136999	-1.574494
H	-5.178816	-1.151438	-2.835627
H	-1.259335	-1.894185	-1.672801
H	-1.238779	3.743371	1.865867
H	-0.765166	4.972724	2.717279
H	0.323097	0.536085	2.691757
H	-0.869760	-0.494948	2.704746
H	-1.916901	2.307127	0.501287
H	-1.448135	1.544408	1.795164
H	2.072399	1.640507	-1.680604
H	2.582559	2.696365	-2.721330
H	1.547360	2.843950	0.303755
H	0.975307	4.020484	1.144792
H	0.372910	-3.802577	1.686025
H	0.884028	-4.152081	3.138951
H	0.552365	-4.559899	-0.309197
H	-0.564850	-3.498296	-0.124398
H	1.883117	1.082600	1.706511

H	2.806212	1.591456	2.790398
H	3.209893	-1.463076	-1.430904
H	2.781613	-1.895107	0.034655
H	-3.942696	0.102338	0.704886
H	-3.615919	1.370578	1.531378
H	4.753853	-0.410018	-3.083698
H	3.623004	0.556355	-2.597532
H	-0.830671	-2.495130	3.181354
H	-2.333902	-1.972650	3.208821
H	2.113561	-2.332099	2.141278
H	2.584300	-0.848885	2.229078
H	4.696829	0.247461	-0.547768
H	4.489094	-0.304281	0.892047
H	-4.872548	-1.956214	3.220807
H	-4.311272	-0.735621	2.436014
H	2.288243	-3.734627	-1.310994
H	2.749208	-5.158262	-0.954977
H	3.305591	3.389523	1.550305
H	4.361943	2.281950	1.444617
H	-3.840393	-1.980640	0.729662
H	2.623815	0.732097	0.016809
H	-2.587785	-1.670365	-0.203155