

Supporting information for

Explicit Polarization: A Quantum Mechanical Framework for Developing Next Generation Force Fields

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Table S1. Computed interaction energies for large water clusters using X-Pol, two-body and three-body variational (VX-Pol, VMB2, VMB3) and embedding (X-Pol, MB2, MB3) many-body expansion with the semiempirical PMO model with and without periodic boundary conditions (p).

	Full QM	VX-Pol	VMB2	VMB3	X-Pol	MB2	MB3
(H ₂ O) ₃₇	-210.7	-135.5	-208.9	-210.7	-117.4	-192.3	-209.8
(H ₂ O) ₆₅	-735.5	-432.6	-720.9	-734.7	-344.8	-602.6	-722.3
p-(H ₂ O) ₁₀₀	-899.3	-905.3	-895.4	-898.6	-724.5	-654.2	-886.2
p-(H ₂ O) ₂₆₇	-2825.0	-1570.0	-2811.3		-1332.2	-2464.9	

3. Coordinates for the cluster of 65 water molecules used in this article.

1.	O	-1.78153	-1.26701	5.88987
2.	H	-2.64057	-1.68672	5.83396
3.	H	-1.10285	-1.82937	5.51798
4.	O	-2.50584	-0.74727	-1.32017
5.	H	-3.26103	-0.48566	-0.78692
6.	H	-2.78343	-1.06928	-2.19172
7.	O	-5.85922	1.35457	-3.48622
8.	H	-6.49362	1.68132	-4.11015
9.	H	-5.85534	0.39369	-3.45516
10.	O	5.66132	1.05309	-2.36212
11.	H	5.65547	0.62006	-1.49934
12.	H	6.52212	1.40337	-2.56070
13.	O	-2.13341	3.38261	5.36163
14.	H	-1.53066	2.63807	5.56499
15.	H	-1.70126	4.22411	5.43045
16.	O	3.22650	-5.70475	-1.51737
17.	H	2.72999	-6.50422	-1.64737
18.	H	3.31376	-5.19798	-2.33098
19.	O	-0.87334	3.26970	-5.65325
20.	H	-0.12983	2.65716	-5.57834
21.	H	-1.67591	2.83250	-5.89823
22.	O	5.54607	-0.92825	2.84200
23.	H	5.97633	-0.08818	2.98747
24.	H	5.00180	-1.21859	3.57305
25.	O	-0.07654	3.74417	-1.96789
26.	H	-0.52053	3.05207	-2.47446
27.	H	0.26682	3.38067	-1.14099
28.	O	3.57199	-4.84561	1.01657
29.	H	3.36462	-5.16790	0.13710
30.	H	3.94295	-5.54196	1.58201
31.	O	-2.23132	5.13573	1.53196
32.	H	-2.73016	5.83043	1.95115
33.	H	-1.63824	5.48298	0.83078
34.	O	5.19112	-2.25890	-3.87680
35.	H	5.66567	-1.87581	-4.60392
36.	H	5.70417	-2.23127	-3.05760
37.	O	1.03307	4.17738	5.21751
38.	H	1.61609	3.40116	5.08866
39.	H	1.05769	4.47723	6.11977
40.	O	-4.03461	-2.81564	5.17244
41.	H	-4.07482	-3.74767	5.32072
42.	H	-4.47788	-2.57859	4.35748
43.	O	4.24638	3.09109	-4.04650
44.	H	4.29481	2.17074	-3.79971
45.	H	4.51302	3.25013	-4.94279

46.	O	-4.06736	-0.18703	2.69577
47.	H	-3.23129	-0.66633	2.72032
48.	H	-4.08204	0.56905	3.28672
49.	O	-0.74809	5.89495	-0.43746
50.	H	-0.72757	5.26380	-1.16501
51.	H	-0.13597	6.60989	-0.56437
52.	O	-3.20157	-5.65832	-2.37308
53.	H	-3.51289	-4.99343	-1.72626
54.	H	-3.87305	-6.30604	-2.56740
55.	O	4.28678	-2.46278	-0.05331
56.	H	5.02339	-2.70624	-0.61303
57.	H	4.06750	-3.15851	0.57226
58.	O	-0.72218	1.20810	5.74189
59.	H	-1.20551	0.39557	5.92516
60.	H	0.02464	1.02640	5.16942
61.	O	-1.64838	1.63233	-2.92101
62.	H	-1.68107	0.95357	-2.25196
63.	H	-2.44776	2.18450	-2.88632
64.	O	-4.14419	-3.83616	-0.73770
65.	H	-4.73311	-3.18983	-1.12214
66.	H	-4.21493	-3.78937	0.21921
67.	O	4.69733	3.78439	-1.25369
68.	H	4.44010	4.48910	-1.85195
69.	H	4.87529	2.98529	-1.73808
70.	O	4.58053	3.38604	3.07504
71.	H	4.01247	3.42839	2.27393
72.	H	4.50732	4.22957	3.52268
73.	O	2.83844	5.60000	3.44644
74.	H	2.66434	5.37935	2.53209
75.	H	2.12912	5.31837	4.02007
76.	O	0.73884	0.66491	3.23444
77.	H	1.18544	0.12253	2.57782
78.	H	0.06245	1.23016	2.86525
79.	O	2.36937	-4.21112	3.56181
80.	H	2.48541	-4.20674	2.61023
81.	H	2.13318	-5.10097	3.82857
82.	O	-0.62936	3.16908	2.67674
83.	H	-0.26570	3.44070	3.51618
84.	H	-1.33283	3.76102	2.39234
85.	O	3.29737	-1.76033	4.31299
86.	H	3.00054	-2.67784	4.25806
87.	H	2.74988	-1.21508	4.87108
88.	O	-1.69767	0.11280	-5.20124
89.	H	-1.54791	0.77718	-4.51787
90.	H	-2.42008	-0.45282	-4.93217
91.	O	-6.21107	-1.46011	-3.47835
92.	H	-6.38173	-1.72708	-2.55720
93.	H	-6.85979	-1.78646	-4.08889

94.	O	-4.22272	2.04999	4.45712
95.	H	-4.52842	1.67779	5.27627
96.	H	-3.45142	2.62777	4.63085
97.	O	0.59246	-1.32366	-5.03331
98.	H	1.34472	-0.74640	-4.91702
99.	H	-0.21498	-0.83810	-5.26097
100.	O	-0.67130	-3.24771	-0.99612
101.	H	-1.50516	-2.78249	-1.01968
102.	H	-0.16289	-3.15857	-1.81887
103.	O	-5.63083	3.05130	2.32570
104.	H	-5.58467	3.98801	2.46806
105.	H	-5.29324	2.57511	3.09869
106.	O	6.09211	-0.19162	0.11999
107.	H	5.52946	-0.83238	0.55861
108.	H	6.32148	0.49349	0.76170
109.	O	2.19772	-1.33950	-1.39592
110.	H	1.74711	-1.99418	-1.94103
111.	H	2.94264	-1.71040	-0.90745
112.	O	0.04676	0.03056	-0.28193
113.	H	0.79270	-0.46385	-0.63288
114.	H	-0.80551	-0.29520	-0.57423
115.	O	0.91196	-3.04858	-3.12572
116.	H	1.61307	-3.65266	-3.36314
117.	H	0.67390	-2.45187	-3.87278
118.	O	3.12671	3.63913	0.93769
119.	H	2.29862	3.20327	0.70669
120.	H	3.71154	3.75859	0.17560
121.	O	-0.27345	-3.19202	4.40024
122.	H	-0.21328	-4.04490	4.80994
123.	H	0.36368	-3.13025	3.68528
124.	O	-1.06046	-5.40777	1.94806
125.	H	-1.14980	-5.75158	1.04760
126.	H	-1.03165	-4.46015	1.96398
127.	O	1.07088	-6.60473	3.07118
128.	H	1.04804	-7.52852	2.85502
129.	H	0.29795	-6.14874	2.69898
130.	O	0.79504	5.03311	-4.30938
131.	H	0.48193	4.74138	-3.45192
132.	H	0.20318	4.71980	-4.99508
133.	O	-2.05852	-2.01217	2.61591
134.	H	-1.26965	-1.96836	2.05986
135.	H	-1.78491	-2.33158	3.47606
136.	O	3.35482	-4.26219	-3.92513
137.	H	3.96541	-3.52086	-3.94283
138.	H	3.27538	-4.68088	-4.79559
139.	O	2.50638	-0.90543	1.83361
140.	H	3.00314	-0.63619	1.07687
141.	H	3.07254	-1.16083	2.57416

142.	O	-6.37142	-2.06209	-0.91588
143.	H	-7.03601	-2.50793	-0.39677
144.	H	-5.90097	-1.35393	-0.42943
145.	O	6.71970	-2.36527	-1.57187
146.	H	7.37159	-3.04482	-1.43418
147.	H	6.84684	-1.58566	-1.01964
148.	O	1.56919	2.19906	-5.14118
149.	H	1.87479	3.02922	-4.80299
150.	H	1.99667	1.46167	-4.68802
151.	O	-0.90790	-6.01570	-0.72471
152.	H	-0.63261	-5.10083	-0.85653
153.	H	-1.63151	-6.20971	-1.31499
154.	O	2.58893	2.13033	4.61724
155.	H	3.40250	2.40278	4.18579
156.	H	2.04632	1.54633	4.07937
157.	O	-3.39936	-1.70179	-3.71837
158.	H	-4.34712	-1.68738	-3.78466
159.	H	-2.99282	-2.53568	-4.03042
160.	O	2.81675	5.58390	-2.40494
161.	H	2.47579	5.63489	-3.30133
162.	H	2.37342	4.88193	-1.94776
163.	O	0.67810	2.52592	0.35570
164.	H	0.22926	2.81580	1.15708
165.	H	0.46098	1.60448	0.13043
166.	O	-5.02681	-0.13898	0.17850
167.	H	-4.68265	-0.09900	1.08404
168.	H	-5.51629	0.66498	-0.06236
169.	O	-3.66734	3.14942	0.17320
170.	H	-3.11316	3.83309	0.54761
171.	H	-4.22029	2.75745	0.84557
172.	O	6.52746	1.70948	2.26089
173.	H	5.84715	2.32347	2.59515
174.	H	7.37848	2.13147	2.22919
175.	O	-6.50726	2.08023	-0.17339
176.	H	-6.44235	2.52449	0.66977
177.	H	-6.33092	2.65334	-0.91810
178.	O	0.33330	-2.59591	1.49372
179.	H	1.08734	-1.99756	1.55582
180.	H	0.14893	-2.86316	0.58818
181.	O	-3.89540	2.98985	-2.49545
182.	H	-4.61964	2.46240	-2.84545
183.	H	-3.86322	3.05122	-1.52708
184.	O	-2.90830	5.54633	-3.33463
185.	H	-3.30649	4.70245	-3.10829
186.	H	-2.10778	5.42929	-3.82778
187.	O	-4.50348	-3.02858	1.96017
188.	H	-3.57904	-2.81372	2.14070
189.	H	-5.01794	-2.22838	1.99627

190.	O	2.87216	0.00597	-3.75783
191.	H	3.71385	-0.42240	-3.88422
192.	H	2.56508	-0.17683	-2.86386
193.	O	-2.36959	-4.07177	-4.43163
194.	H	-2.53877	-4.73978	-3.74852
195.	H	-1.71316	-4.31454	-5.05910