Supporting Information for:

Electrostatically Embedded Many-Body Correlation Energy, with Applications to the Calculation of Accurate Second-Order Møller-Plesset Perturbation Theory Energies for Large Water Clusters

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Table S1: Calculated[a] Binding Energies[b] (in kcal/mol) for Cluster Containing 5 to 20 Water Molecules

Structure	Full MP2[c]	PA	3B	EE-PA	EE-3B	PA-CE	3B-CE	EE-PA-CE	EE-3B-CE
5	33.52	26.76	32.76	33.11	33.46	33.42	33.40	33.55	33.50
6-cage	42.67	36.41	42.39	42.24	42.69	42.56	42.64	42.72	42.69
6-prism	42.90	36.65	42.58	42.56	42.96	42.79	42.87	42.98	42.95
7	53.71	45.35	53.19	53.25	53.74	53.56	53.64	53.77	53.74
8	68.40	57.81	67.94	67.70	68.53	68.17	68.37	68.40	68.48
9	77.08	64.47	76.20	76.40	77.11	76.94	76.98	77.14	77.11
10	87.80	73.49	86.79	87.04	87.87	87.64	87.68	87.87	87.84
11	93.67	80.06	93.35	92.92	93.94	93.39	93.71	93.75	93.85
12	110.63	94.04	110.34	109.81	111.12	110.42	110.82	110.71	110.95
13	115.71	98.54	115.34	114.91	116.17	115.37	115.83	115.77	116.00
14	116.76	100.13	115.91	115.76	116.97	116.70	116.66	116.95	116.87
15	141.23	118.37	139.89	140.20	141.42	140.92	141.04	141.38	141.35
17	159.16	136.53	159.16	158.16	160.09	158.92	159.58	159.32	159.77
18	166.06	143.11	166.14	165.10	167.03	165.84	166.49	166.26	166.70
19	182.01	153.20	180.54	180.66	182.43	181.58	181.83	182.18	182.29
20	196.02	167.05	195.99	194.79	197.29	195.66	196.62	196.17	196.87

[a] All calculations use the MP2/aug´-cc-pVTZ level of theory (the aug-cc-pVTZ basis set on oxygen and the cc-pVTZ basis set on hydrogen).

[b] $E_{\text{bind, X}} = n*E_{\text{monomer}} - E_{\text{cluster, X}}$ where n is the number of water molecules in the cluster, E_{monomer} is the MP2/aug´-cc-pVTZ single-point energy of a gas-phase water molecule, and $E_{\text{cluster, X}}$ is the energy of the cluster predicted by method X (X = MP2, PA, EE-PA-CE, etc.)

[c] Full MP2 is the binding energy obtained when the energy of the entire cluster is calculated at the MP2 level of theory – no many-body approximation is employed.