Supporting Information

ABEEM/MM OH^- Models for $OH^-(H_2O)_n$ Clusters and Aqueous OH^-: Structures, Charge Distributions, and Binding Energies

Hua Shi[†,‡] , Li-Dong Gong[†]*, Cui Liu[†], Li-Nan Lu[†], and Zhong-Zhi Yang[†]*

[†]School of Chemistry and Chemical Engineering, Liaoning Normal University, Dalian, 116029, People's Republic of China

[‡]School of Marine Science and Environment, Dalian Ocean University, Dalian 116023, People's Republic of China

Corresponding authors E-mail address:

gongjw@lnnu.edu.cn (Li-Dong Gong)

zzyang@lnnu.edu.cn (Zhong-Zhi Yang)

Tel: +86 411-82159607

1. THE THEORETICAL FORMULAS

1.1. The Theoretical Formulas of the ABEEM/MM-I.

$$\chi_{\mathrm{O(OH^-)}} = \chi_{\mathrm{H(OH^-)}} = \chi_{\mathrm{O\text{-}H(OH^-)}} = \bar{\chi}_{\mathrm{OH^-}} \quad \text{(S1)}$$

$$\chi_{Ii} = \chi_{I(i-j)} = \chi_{I(lp)} = \cdots = \bar{\chi}_I \quad \text{(S2)}$$

$$\chi_{Ji} = \chi_{J(i-j)} = \chi_{J(lp)} = \cdots = \bar{\chi}_J \quad \text{(S3)}$$

$$\vdots$$

Eqs. (S1)-(S3) are the electronegativity equalization equations of the ABEEM/MM-I model. Eq. (S1) is the electronegativity equalization equations of the OH^-, and the remaining equations are those of the water molecules. Eq. (S1) represents that the electronegativities of O atom, H atom, and O-H bond of OH^- are equal to the electronegativity of the OH^-. Herein, $\chi_{\mathrm{O(OH^-)}}$, $\chi_{\mathrm{H(OH^-)}}$, and $\chi_{\mathrm{O\text{-}H(OH^-)}}$ are the electronegativities of O atom, H atom, and O-H bond of the OH^-, and $\bar{\chi}_{\mathrm{OH^-}}$ is the global electronegativity of the OH^-. Eq. (S2) represents that the electronegativities of each atom, each bond, and each lone-pair electron in water molecule *I* are equal to the electronegativity of the water molecule *I*. Herein, χ_{Ii}, $\chi_{I(i\text{-}j)}$, and $\chi_{I(lp)}$ are the electronegativities of atom *i*, bond *i-j*, and lone-pair electron *lp* in water molecule *I*, and $\bar{\chi}_I$ is the global electronegativity of water molecule *I*. The remaining equations are the electronegativity equalization equations of other water molecules.

$$q_{\mathrm{O(OH^-)}} + q_{\mathrm{H(OH^-)}} + q_{\mathrm{O\text{-}H(OH^-)}} = -1$$

(S4)

$$\sum_{i}^{N_i} q_{Ii} + \sum_{i-j}^{N_{i-j}} q_{I(i-j)} + \sum_{lp}^{N_{lp}} q_{I(lp)} = 0 \quad \text{(S5)}$$

$$\sum_{i}^{N_i} q_{Ji} + \sum_{i-j}^{N_{i-j}} q_{J(i-j)} + \sum_{lp}^{N_{lp}} q_{J(lp)} = 0 \tag{S6}$$

$$\vdots$$

Eqs. (S4)-(S6) are charge conservation functions of the ABEEM/MM-I model. Eq. (S4) represents that the total charge of the hydroxide ion is constrained to be -1.0*e*. Herein, $q_{\text{O(OH}^-)}$, $q_{\text{H(OH}^-)}$, and $q_{\text{O-H(OH}^-)}$ are the charges of O atom, H atom, and O-H bond of OH^-. Eq. (S5) represents that the total charge of the water molecule *I* is zero. Herein, q_{Ii}, $q_{I(i\text{-}j)}$, and $q_{I(lp)}$ are the charges of atom *i*, bond *i-j*, and lone-pair electron *lp* in water molecule *I*. The remaining equations represent that other water molecules are electric neutral.

1.2. The Theoretical Formulas of the ABEEM/MM-II.

$$\chi_{\text{O(OH}^-)} = \chi_{\text{H(OH}^-)} = \chi_{\text{O-H(OH}^-)} = \chi_{Fi} = \chi_{F(i-j)} = \chi_{F(lp)} = \cdots = \overline{\chi}_L \tag{S7}$$

$$\chi_{Ii} = \chi_{I(i-j)} = \chi_{I(lp)} = \cdots = \overline{\chi}_I \tag{S8}$$

$$\chi_{Ji} = \chi_{J(i-j)} = \chi_{J(lp)} = \cdots = \overline{\chi}_J \tag{S9}$$

$$\vdots$$

Eqs. (S7)-(S9) are the electronegativity equalization equations of the ABEEM/MM-II model. Eq. (S7) is the electronegativity equalization equation of the OH^- and its first-shell water molecules, and the remaining equations are those of the external-shell water molecules. Eq. (S7) represents that the electronegativities of each atom, each bond, and each lone-pair electron of the OH^- and water molecules in the first hydration shell are equal to the global electronegativity of the first shell including the OH^-. Herein, χ_{Fi}, $\chi_{F(i-j)}$, and $\chi_{F(lp)}$ are the electronegativities of atom *i*, bond *i-j*, and lone-pair electron *lp* of the first-shell water molecule *F*. Eq. (S8) represents that the electronegativities of each atom, each bond, and each lone-pair electron in the external-shell water molecule *I* are equal to the electronegativity of the water molecule *I*. The remaining equations are the electronegativity equalization equations of other external-shell water molecules.

$$q_{\mathrm{O(OH^-)}} + q_{\mathrm{H(OH^-)}} + q_{\mathrm{O\text{-}H(OH^-)}} + \sum_{F}^{M}\left(\sum_{i}^{N_i} q_{Fi} + \sum_{i-j}^{N_{i-j}} q_{F(i-j)} + \sum_{lp}^{N_{lp}} q_{F(lp)}\right) = -1 \qquad \text{(S10)}$$

$$\sum_{i}^{N_i} q_{Ii} + \sum_{i-j}^{N_{i-j}} q_{I(i-j)} + \sum_{lp}^{N_{lp}} q_{I(lp)} = 0 \qquad \text{(S11)}$$

$$\sum_{i}^{N_i} q_{Ji} + \sum_{i-j}^{N_{i-j}} q_{J(i-j)} + \sum_{lp}^{N_{lp}} q_{J(lp)} = 0 \qquad \text{(S12)}$$

$$\vdots$$

Eqs. (S10)-(S12) are charge conservation functions of the ABEEM/MM-II model. Eq. (S10) represents that the total charge of the OH^- and its first-shell water molecules is constrained to be -1.0*e*. Herein, q_{Fi}, $q_{F(i\text{-}j)}$, and $q_{F(lp)}$ are the charges of atom *i*, bond *i-j*, and lone-pair electron *lp* in first-shell water molecule *F*. Eq. (S11) represents that the total charge of the external-shell water molecule *I* is zero. The remaining equations represent that other external-shell water molecules are electric neutral.

2. Parameters of the ABEEM/MM

Parameters of water molecule in external shells are as same as before[1]. The parameters of the OH^- and water molecules in its hydration first shell are listed in the following. The parameters of the ABEEM/MM-I and the ABEEM/MM-II are listed in Table S1 and S2, respectively. The parameters of the optimized correction functions of hydrogen bonds are listed in Table S3.

Table S1. The ABEEM/MM-I Parameters

	χ^*	$2\eta^*$	C	D	r_{OH}(Å)	k_{OH}	θ	k_θ	σ (Å)	ε (kcal/mol)
H (OH^-)	5.023	60.000							1.500	0.030
O (OH^-)	1.700	0.500							3.200	0.250
O-H (OH^-)	8.000	50.000			0.9670	529.6				
H (firstshell-H_2O)	2.123	12.000	2.161						2.240	0.005
O (firstshell-H_2O)	3.700	1.000	11.493	5.312					3.051	0.044
O-H (firstshell-H_2O)	5.136	24.767	2.161	11.493	0.9830	535.6				
H-O-H (firstshell-H_2O)							104.52	34.05		
lp (firstshell-H_2O)	3.700	0.500	1.612							

Table S2. The ABEEM/MM-II Parameters

	χ^*	$2\eta^*$	C	D	r_{OH}(Å)	k_{OH}	θ	k_θ	σ(Å)	ε(kcal/mol)
H (OH^-)	2.023	13.220							1.500	0.0200
O (OH^-)	1.685	8.527							3.420	0.2512
O-H (OH^-)	10.640	4.470			0.9730	530.6				
H (firstshell-H_2O)	2.023	8.840	2.161						2.240	0.0020
O (firstshell-H_2O)	3.373	0.100	11.493	5.312					3.051	0.0440
O-H (firstshell-H_2O)	5.136	38.500	2.161	11.493	0.9830	533.6				
H-O-H (firstshell-H_2O)							104.52	34.05		
lp (firstshell-H_2O)	3.878	13.950	5.312							

Table S3. The Optimized Correction Functions of Hydrogen Bonds

		A	B	U	V
ABEEM/MM-I	$k_{HB(R_{O(OH^-),I(H)})}$	1.1700	0.1057	1.7500	0.0430
	$k_{HB(R_{IH,J(lp)})}$	0.6831	0.0894	1.1510	0.0697
ABEEM/MM-II	$k_{HB(R_{O(OH^-),I(H)})}$	0.9477	0.0797	1.8000	0.0430
	$k_{HB(R_{IH,J(lp)})}$	0.6210	0.0813	1.1510	0.0697

[a] $k_{HB(R_{O(OH^-),I(H)})}$ is the optimized correction function of the hydrogen bond between the oxygen atom of OH^- and the hydrogen atom of a first-shell water molecule in the HBIR.

[b] $k_{HB(R_{IH,J(lp)})}$ is the optimized correction function of the hydrogen bond between the hydrogen atom of a first-shell water molecule and the lone-pair electron *lp* of an external-shell water molecule in the HBIR.

3. The Results of Optimized Structures ($R_{\text{O-H}}$, $\bar{R}_{\text{O}\cdots\text{H}}$, $\bar{\theta}_{\text{H}\cdots\text{O}\cdots\text{H}}$, and $\bar{\theta}_{\text{O}\cdots\text{H-O}}$) and Binding Energies for the $OH^-(H_2O)_n$ (*n* = 1-8) Clusters.

Table S4. Optimized Structures ($R_{\text{O-H}}$, $\bar{R}_{\text{O}\cdots\text{H}}$, $\bar{\theta}_{\text{H}\cdots\text{O}\cdots\text{H}}$, and $\bar{\theta}_{\text{O}\cdots\text{H-O}}$) of the $OH^-(H_2O)_n$ (*n* = 1-8) Clusters Obtained from the Two ABEEM/MM Models and the *Ab Initio* Calculations

Cluster	$R_{\text{O-H}}$ [a] (Å)			$\bar{R}_{\text{O}\cdots\text{H}}$ [b]			$\bar{\theta}_{\text{H}\cdots\text{O}\cdots\text{H}}$ [c]			$\bar{\theta}_{\text{O}\cdots\text{H-O}}$ [d] (º)		
	MP2/aug-cc-pVDZ	ABEEM/MM-I	ABEEM/MM-II	MP2/aug-cc-pVDZ	ABEEM/MM-I	ABEEM/MM-II	MP2/aug-cc-pVDZ	ABEEM/MM-I	ABEEM/MM -II	MP2/aug-cc-pVDZ	ABEEM/MM-I	ABEEM/MM -II
1 (1+0)	0.970	0.965	0.968	1.483	1.534	1.571				176.2	177.2	176.8
2 (2+0)	0.969	0.966	0.965	1.615	1.629	1.646	85.4	85.0	84.5	170.4	171.1	171.2
3-*a* (3+0)	0.966	0.964	0.953	1.709	1.711	1.729	84.7	84.6	83.8	160.0	160.5	161.3
3-*b* (2+1)	0.968	0.963	0.963	1.549	1.568	1.576	107.0	106.6	106.2	173.3	173.8	173.8
4-*a* (4+0)	0.967	0.967	0.972	1.774	1.771	1.858	75.1	75.1	71.2	162.5	162.8	167.4
4-*b* (3+1)	0.966	0.963	0.957	1.680	1.685	1.695	85.9	85.5	85.2	161.1	161.9	162.2
4-*c* (3+1)	0.966	0.964	0.961	1.670	1.675	1.685	97.7	97.5	97.1	168.2	168.6	168.8
5-*a* (5+0)	0.969	0.969	0.971	1.845	1.782	1.843	67.2	67.9	67.2	168.6	169.3	168.7
5-*b* (4+1)	0.968	0.967	0.967	1.744	1.743	1.746	79.1	79.1	79.1	167.4	167.6	167.6
5-*c* (4+1)	0.967	0.967	0.967	1.730	1.729	1.733	79.9	79.9	79.9	168.8	169.3	169.3
5-*d* (4+1)	0.967	0.968	0.965	1.755	1.753	1.758	79.6	79.6	79.5	165.6	166.0	166.0
5-*e* (3+2)	0.968	0.967	0.968	1.616	1.626	1.627	110.5	110.4	110.4	175.4	175.7	175.6
6-*a* (5+1)	0.969	0.970	0.970	1.859	1.854	1.856	71.6	71.6	71.7	164.4	164.6	164.4
6-*b* (3+3)	0.966	0.963	0.960	1.659	1.666	1.674	98.2	98.0	97.7	164.9	165.1	165.4
6-*c* (3+3)	0.967	0.966	0.963	1.635	1.642	1.647	100.3	100.0	99.9	169.9	171.0	170.5
6-*d* (3+3)	0.968	0.968	0.966	1.585	1.594	1.596	108.8	108.7	108.7	178.3	179.2	179.0
7-*a* (4+3)	0.968	0.968	0.966	1.741	1.740	1.744	80.9	80.9	80.8	168.2	168.7	168.6
7-*b* (3+4)	0.967	0.966	0.964	1.637	1.643	1.647	99.4	99.2	99.1	169.1	170.0	169.6
7-*c* (4+3)	0.968	0.968	0.965	1.741	1.740	1.746	82.5	82.4	82.3	166.1	166.3	166.5
8-*a* (3+5)	0.967	0.964	0.962	1.612	1.628	1.628	100.4	100.0	100.0	170.1	170.7	170.4
8-*b* (4+4)	0.968	0.967	0.966	1.736	1.736	1.739	86.3	86.3	86.2	170.1	169.9	169.9

MAD[e]		0.002	0.004		0.011	0.018		0.2	0.5		0.5	0.7

[a] $R_{\text{O-H}}$ is the bond length of OH^-. [b] $\overline{R}_{\text{O}\cdots\text{H}}$ is the average hydrogen bond length formed by the oxygen atom of OH^- and the hydrogen atom of a first-shell water molecules. [c] $\overline{\theta}_{\text{H}\cdots\text{O}\cdots\text{H}}$ is the average angle between two neighboring hydrogen bonds in the first shell. [d] $\overline{\theta}_{\text{O}\cdots\text{H-O}}$ is the average hydrogen bond angle formed by the O atom of OH^- and the H-O bond of a first-shell water molecule**.** [e]MAD is the mean absolute deviation of the results of the ABEEM/MM models compared to those of MP2/aug-cc-pVDZ.

Table S5. Optimized Structures ($R_{\text{O-H}}$, $\bar{R}_{\text{O}\cdots\text{H}}$, $\bar{\theta}_{\text{H}\cdots\text{O}\cdots\text{H}}$, and $\bar{\theta}_{\text{O}\cdots\text{H-O}}$) of the $OH^-(H_2O)_n$ (n = 1-8) Clusters Obtained from the OPLS/AA-FF, the OPLS-SMOOTH/AA-FF, and the *Ab Initio* Calculations

Cluster	$R_{\text{O-H}}$ [a] (Å)			$\bar{R}_{\text{O}\cdots\text{H}}$ [b]			$\bar{\theta}_{\text{H}\cdots\text{O}\cdots\text{H}}$ [c]			$\bar{\theta}_{\text{O}\cdots\text{H-O}}$ [d]		
	MP2/aug-cc-pVDZ	OPLS/AA-FF	OPLS-SMOOTH/AA-FF	MP2/aug-cc-pVDZ	OPLS/AA-FF	OPLS-SMOOTH/AA-FF	MP2/aug-cc-pVDZ	OPLS/AA-FF	OPLS-SMOOTH/AA-FF	MP2/aug-cc-pVDZ	OPLS/AA-FF	OPLS-SMOOTH/AA-FF
1 (1+0)	0.970	0.947	0.948	1.483	1.609	1.554				176.2	165.1	166.0
2 (2+0)	0.969	0.950	0.950	1.615	1.639	1.595	85.4	75.6	77.7	170.4	164.4	165.2
3-*a* (3+0)	0.966	0.952	0.953	1.709	1.667	1.630	84.7	78.2	79.9	160.0	162.1	163.1
3-*b* (2+1)	0.968	0.951	0.951	1.549	1.589	1.533	107.0	95.0	99.3	173.3	169.4	169.9
4-*a* (4+0)	0.967	0.955	0.956	1.774	1.682	1.654	75.1	72.4	73.6	162.5	163.9	164.9
4-*b* (3+1)	0.966			1.680			85.9			161.1		
4-*c* (3+1)	0.966	0.954	0.954	1.670	1.627	1.586	97.7	90.9	92.4	168.2	167.2	167.7
5-*a* (5+0)	0.969	0.958	0.959	1.845	1.698	1.685	67.2	67.0	67.7	168.6	168.2	168.8
5-*b* (4+1)	0.968	0.956	0.956	1.744	1.659	1.629	79.1	75.9	77.2	167.4	168.0	168.6
5-*c* (4+1)	0.967	0.956	0.957	1.730	1.656	1.625	79.9	76.2	77.5	168.8	168.0	168.6
5-*d* (4+1)	0.967	0.956	0.957	1.755	1.659	1.628	79.6	79.9	81.1	165.6	167.2	167.9
5-*e* (3+2)	0.968	0.956	0.956	1.616	1.593	1.543	110.5	104.0	105.5	175.4	173.6	174.0
6-*a* (5+1)	0.969	0.959	0.959	1.859	1.693	1.673	71.6	75.1	76.1	164.4	166.2	166.8
6-*b* (3+3)	0.966	0.955	0.956	1.659	1.595	1.545	98.2	94.1	95.9	164.9	172.5	172.8
6-*c* (3+3)	0.967			1.635			100.3			169.9		
6-*d* (3+3)	0.968			1.585			108.8			178.3		
7-*a* (4+3)	0.968			1.741			80.9			168.2		
7-*b* (3+4)	0.967	0.955	0.955	1.637	1.608	1.562	99.4	100.7	102.2	169.1	169.9	170.6
7-*c* (4+3)	0.968	0.957	0.958	1.741	1.640	1.606	82.5	82.6	83.5	166.1	169.4	170.2
8-*a* (3+5)	0.967			1.612			100.4			170.1		
8-*b* (4+4)	0.968	0.959	0.960	1.736	1.622	1.586	86.3	89.3	90.4	170.1	175.1	175.3
MAD[e]		0.013	0.012		0.346	0.102		4.2	3.5		3.1	3.2

[a] $R_{\text{O-H}}$ is the bond length of OH^-. [b] $\bar{R}_{\text{O}\cdots\text{H}}$ is the average hydrogen bond length formed by the oxygen atom of OH^- and the hydrogen atom of a first-shell water molecules. [c] $\bar{\theta}_{\text{H}\cdots\text{O}\cdots\text{H}}$ is the average angle between two neighboring hydrogen bonds in the first shell. [d] $\bar{\theta}_{\text{O}\cdots\text{H-O}}$ is the average hydrogen bond angle formed by the O atom of OH^- and the H-O bond of a first-shell water molecule**.** [e]MAD is the mean absolute deviation of the results of the OPLS/AA-FF and OPLS-SMOOTH/AA-FF compared to those of MP2/aug-cc-pVDZ.

Table S6. Binding Energies (in kcal/mol) of $OH^{-}(H_2O)_n$ (*n* = 1-8) Obtained from the Two ABEEM/MM Models, the OPLS/AA-FF, the OPLS-SMOOTH/AA-FF, and the *Ab Initio* Calculations

Cluster	ABEEM/MM-I	ABEEM/MM-II	OPLS/AA-FF	OPLS-SMOOTH/AA-FF	MP2/aug-cc-pVDZ[a]
1 (1+0)	-22.88	-24.49	-24.36	-24.42	-23.46
2 (2+0)	-41.99	-36.29	-47.43	-47.29	-41.47
3-*a* (3+0)	-58.59	-56.16	-69.61	-69.16	-57.09
3-*b* (2+1)	-54.35	-56.59	-63.75	-63.68	-56.32
4-*a* (4+0)	-74.49	-69.39	-89.77	-88.93	-71.01
4-*b* (3+1)	-68.42	-75.42			-68.64
4-*c* (3+1)	-68.34	-72.76	-85.19	-84.77	-69.60
5-*a* (5+0)	-87.67	-78.59	-106.38	-105.05	-80.71
5-*b* (4+1)	-85.43	-81.75	-103.55	-102.65	-82.50
5-*c* (4+1)	-83.82	-81.90	-103.08	-102.21	-82.53
5-*d* (4+1)	-84.13	-82.89	-104.12	-103.24	-83.51
5-*e* (3+2)	-80.45	-79.72	-97.46	-97.11	-82.35
6-*a* (5+1)	-98.56	-95.87	-122.00	-120.55	-93.95
6-*b* (3+3)	-97.18	-87.23	-113.04	-112.42	-92.71
6-*c* (3+3)	-87.19	-97.05			-94.02
6-*d* (3+3)	-84.53	-83.21			-91.88
7-*a* (4+3)	-102.39	-116.63			-105.07
7-*b* (3+4)	-100.44	-111.47	-120.85	-119.73	-105.78
7-*c* (4+3)	-106.00	-92.39	-126.71	-125.58	-103.62
8-*a* (3+5)	-121.77	-122.91			-113.56
8-*b* (4+4)	-126.76	-123.54	-142.85	-141.44	-115.63
MRE[b]	4.07%	5.09%	21.20%	20.35%	

[a]Binding energies were calculated with CP and ZPE corrections.
[b]MRE is the mean relative error of the results of the ABEEM/MM models, the OPLS/AA-FF, and the OPLS-SMOOTH/AA-FF compared to those of MP2/aug-cc-pVDZ.

4. The Results of Optimized Structures ($R_{O\text{-}H}$, $\bar{R}_{O\cdots H}$, $\bar{\theta}_{H\cdots O\cdots H}$, and $\bar{\theta}_{O\cdots H\text{-}O}$) and Binding Energies for the Larger Clusters.

Table S7. Optimized Structures ($R_{O\text{-}H}$, $\bar{R}_{O\cdots H}$, $\bar{\theta}_{H\cdots O\cdots H}$, and $\bar{\theta}_{O\cdots H\text{-}O}$) of the Larger Clusters Obtained from the ABEEM/MM-I Model and the QM Calculations

Cluster	$R_{O\text{-}H}$ [a] (Å)		$\bar{R}_{O\cdots H}$ [b] (Å)		$\bar{\theta}_{H\cdots O\cdots H}$ [c] (°)		$\bar{\theta}_{O\cdots H\text{-}O}$ [d] (°)	
	QM	ABEEM/MM-I	QM	ABEEM/MM-I	QM	ABEEM/MM-I	QM	ABEEM/MM-I
10(4+6)	0.969	0.970	1.738	1.736	83.2	83.2	170.0	170.0
15(3+12)	0.964	0.961	1.573	1.586	100.5	100.0	167.3	168.4
23(3+20)	0.965	0.963	1.549	1.559	107.0	106.9	173.4	173.4
MAD[f]		0.002		0.008		0.2°		0.4°

[a] $R_{O\text{-}H}$ is the bond length of OH^-. [b] $\bar{R}_{O\cdots H}$ is the average hydrogen bond length formed by the oxygen atom of OH^- and the hydrogen atom of a first-shell water molecules. [c] $\bar{\theta}_{H\cdots O\cdots H}$ is the average angle between two neighboring hydrogen bonds in the first shell. [d] $\bar{\theta}_{O\cdots H\text{-}O}$ is the average hydrogen bond angle formed by the O atom of OH^- and the H-O bond of a first-shell water molecule**.** [e] The QM results of $OH^-(H_2O)_{10}$ are from MP2/aug-cc-pVDZ calculation and the results of $OH^-(H_2O)_n$ (n = 15, 23) are from B3LYP/6-31++G(d,p) calculations. [f] MAD is the mean absolute deviation of the results of the ABEEM/MM-I model compared to those of QM results.

Table S8. Binding Energies (in kcal/mol) of $OH^-(H_2O)_n$ (n = 10, 15, 23) from the ABEEM/MM-I Model, the OPLS/AA-FF, the OPLS-SMOOTH/AA-FF, and the QM Calculations

Cluster	ABEEM/MM-I	OPLS/AA-FF	OPLS-SMOOTH/AA-FF	QM[a]
10(4+6)	-127.5	-161.8	-159.7	-137.6
15(3+12)	-180.3			-188.9
23(3+20)	-293.7			-270.9
MRE[b]	6.67%			

[a]Binding energies were calculated with CP and ZPE corrections.
[b]MRE is the mean relative error of the results of the ABEEM/MM-I model compared to those of QM results.

REFERENCES

1. Yang, Z.-Z.; Wu, Y.; Zhao, D.-X. Atom-Bond Electronegativity Equalization Method Fused into Molecular Mechanics. I. A Seven-Site Fluctuating Charge and Flexible Body Water Potential Function for Water Clusters. *J. Chem. Phys.* **2004,** *120*, 2541-2557