Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
This journal is © the Owner Societies 2018

Supplementary Information: New tricks for old dogs: Improving the accuracy of biomolecular force fields by pair-specific corrections to non-bonded interactions

Jejoong Yoo[†,‡] and Aleksei Aksimentiev[*,†]

[†]*Center for the Physics of Living Cells, Department of Physics, University of Illinois at Urbana–Champaign, 1110 West Green Street, Urbana, Illinois 61801*

[‡]*Center for Self-assembly and Complexity, Institute for Basic Science, Pohang, 37363, Republic of Korea*

E-mail: aksiment@illinois.edu

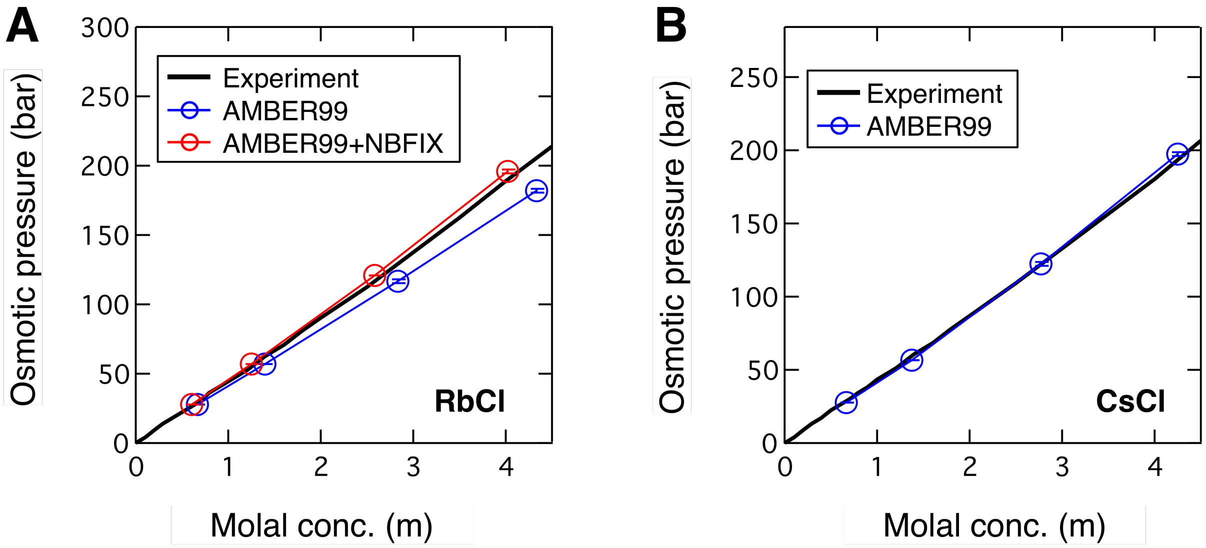

Figure S1: Validation and calibration of Rb^+–Cl^- (A) and Cs^+–Cl^- (B) ion pair interactions for the AMBER ff99 force fields using osmotic pressure simulations. Standard ion parameters optimized for the TIP3P water were taken from Joung and Cheatham.[1] The simulation method for computing osmotic pressure was similar to that used in Ref. 2 and 3. NBFIX corrections, if necessary, were applied to the Lennard-Jones σ parameters for cation–anion atom pairs. Experimental data were taken from Ref. 4. See Table 3 for the changes in σ parameters.

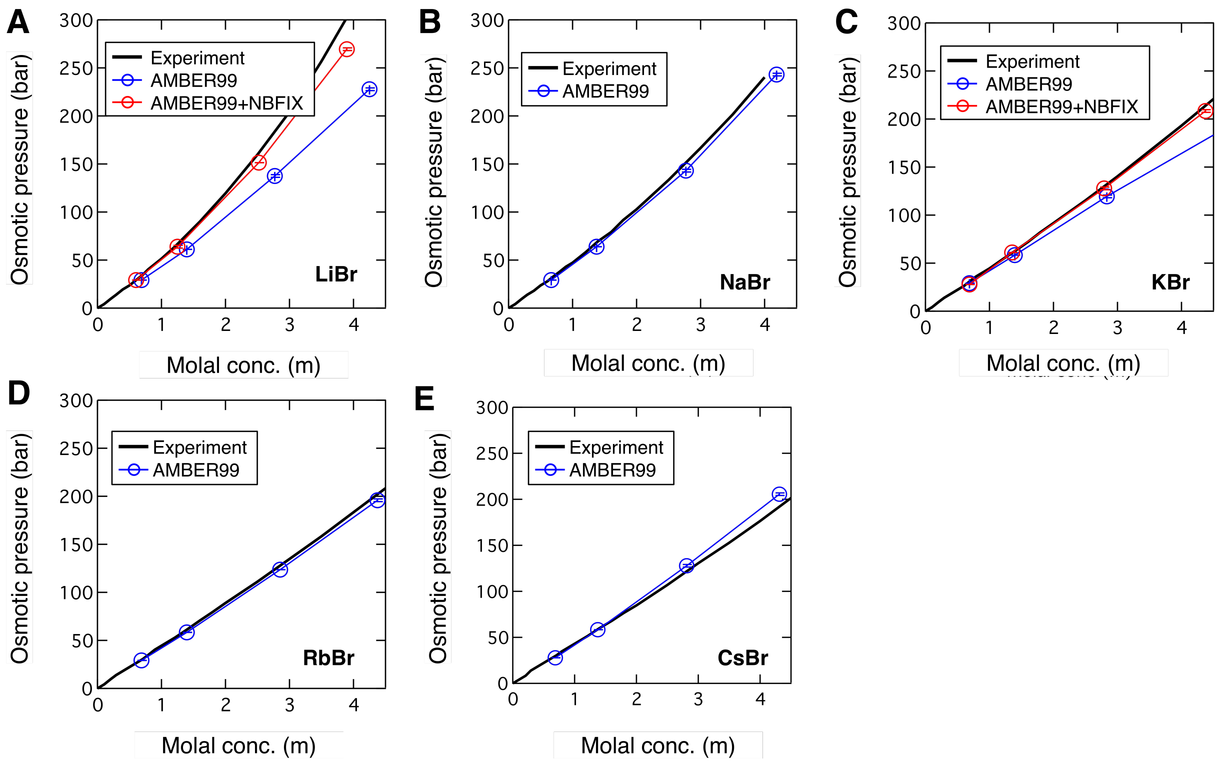

Figure S2: Validation and calibration of Li$^+$–Br$^-$ (A), Na$^+$–Br$^-$ (B), K$^+$–Br$^-$ (C), Rb$^+$–Br$^-$ (D), and Cs$^+$–Br$^-$ (E) ion pair interactions for the AMBER ff99 force fields using osmotic pressure simulations. Standard ion parameters optimized for the TIP3P water were taken from Joung and Cheatham.[1] The simulation method for computing osmotic pressure was similar to that used in Ref. 2 and 3. NBFIX corrections, if necessary, were applied to the Lennard-Jones σ parameters for cation–anion atom pairs. Experimental data were taken from Ref. 4. See Table 3 for the changes in σ parameters.

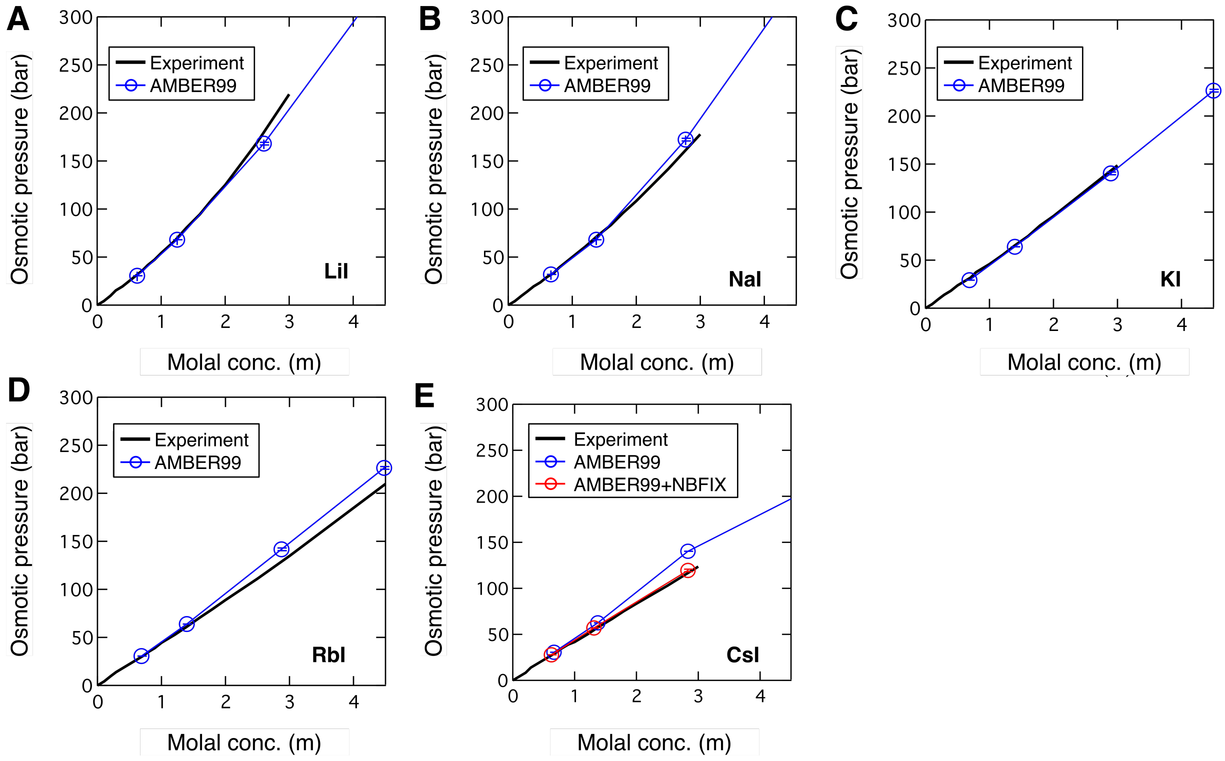

Figure S3: Validation and calibration of Li$^+$–I$^-$ (A), Na$^+$–I$^-$ (B), K$^+$–I$^-$ (C), Rb$^+$–I$^-$ (D), and Cs$^+$–I$^-$ (E) ion pair interactions for the AMBER ff99 force fields using osmotic pressure simulations. Standard ion parameters optimized for the TIP3P water were taken from Joung and Cheatham.[1] The simulation method for computing osmotic pressure was similar to that used in Ref. 2 and 3. NBFIX corrections, if necessary, were applied to the Lennard-Jones σ parameters for cation–anion atom pairs. Experimental data were taken from Ref. 4. See Table 3 for the changes in σ parameters.

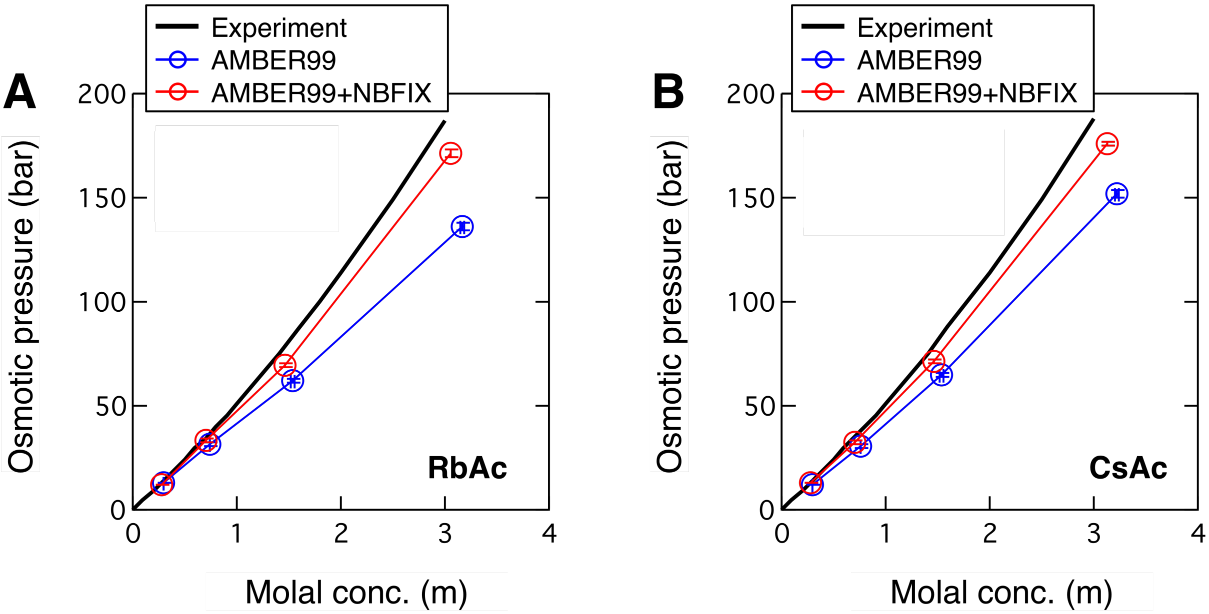

Figure S4: Validation and calibration of Rb^+–Ac^- (A) and Cs^+–Ac^- (B) ion pair interactions for the AMBER ff99 force fields using osmotic pressure simulations. Standard ion parameters optimized for the TIP3P water were taken from Joung and Cheatham.[1] Standard parameters for acetate were taken from AMBER ff99. The simulation method for computing osmotic pressure was similar to that used in Ref. 2 and 3. NBFIX corrections, if necessary, were applied to the Lennard-Jones σ parameters for cation–acetate oxygen atom pairs. Experimental data were taken from Ref. 4. See Table 3 for the changes in σ parameters.

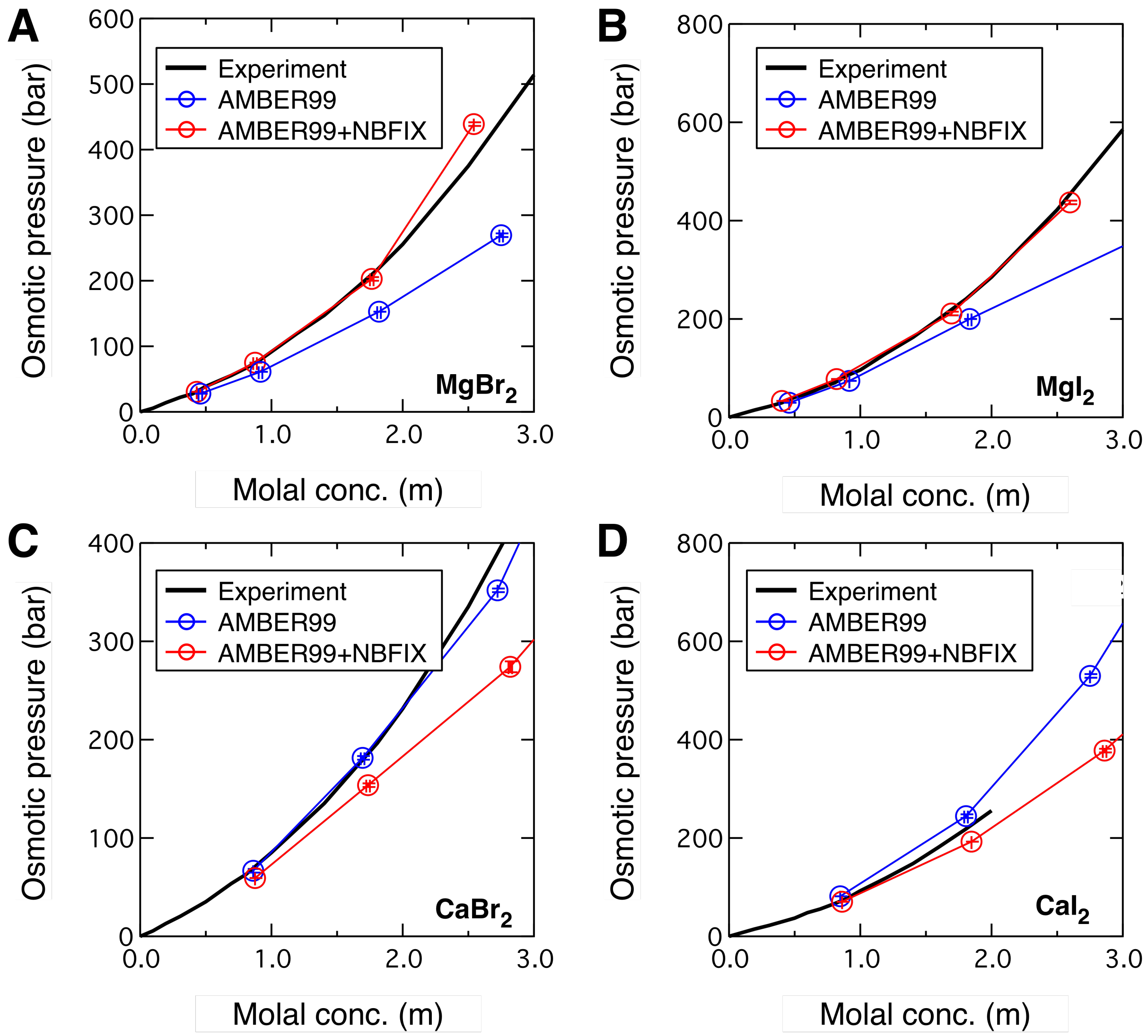

Figure S5: Validation and calibration of Mg^{2+}–Br^- (A), Mg^{2+}–I^- (B), Ca^{2+}–Br^- (C), and Ca^{2+}–I^- (D) ion pair interactions for the AMBER ff99 force fields using osmotic pressure simulations. Standard parameters for Mg^{2+} and Ca^{2+} were taken from the CHARMM36 force field.[5] In all calibration simulations that used NBFIX, Mg^{2+} and Ca^{2+} ions were in the hexahydrate and heptahydrate forms, respectively; the dipole moment of the water molecules forming hexa- and heptahydrates was adjusted to account for the polarization effect.[2] Standard parameters for Br^- and I^- were taken from Joung and Cheatham.[1] The simulation method for computing osmotic pressure was similar to that used in Ref. 2 and 3. NBFIX corrections, if necessary, were applied to the Lennard-Jones R_{min} parameter of the hexa- or heptahydrate water oxygen – anion atom pairs. Experimental data were taken from Ref. 4. See Table 3 for the changes in σ parameters.

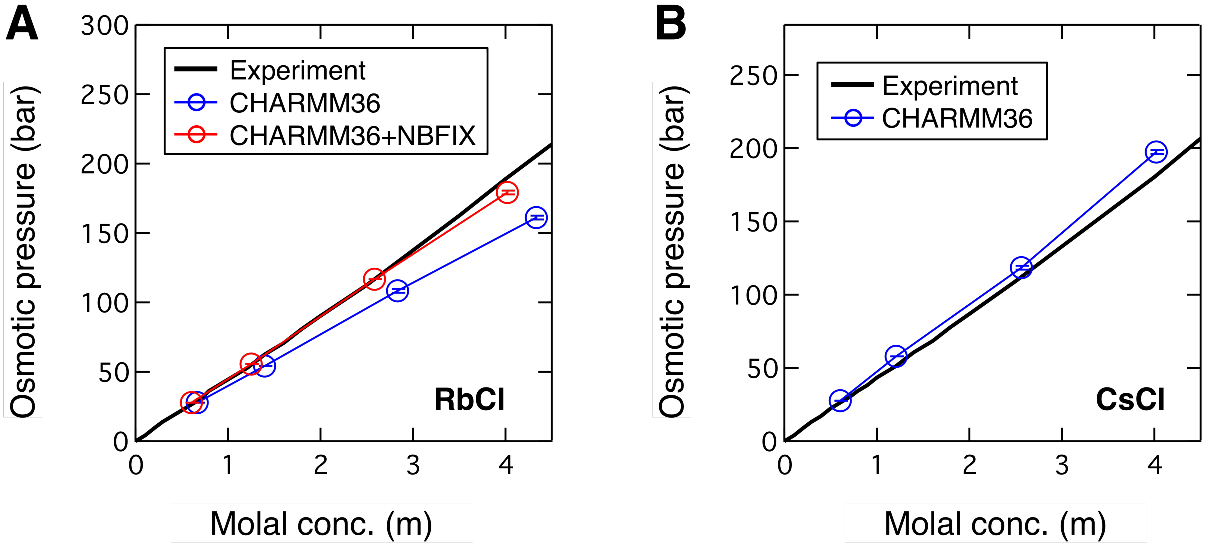

Figure S6: Validation and calibration of Rb^+–Cl^- (A) and Cs^+–Cl^- (B) ion pair interactions for the CHARMM36 force field using osmotic pressure simulations. The simulation method for computing osmotic pressure was similar to that used in Ref. 2 and 3. NBFIX corrections, if necessary, were applied to the Lennard-Jones R_{min} parameters for cation–anion atom pairs. Experimental data were taken from Ref. 4. See Table 4 for the changes in R_{min} parameters.

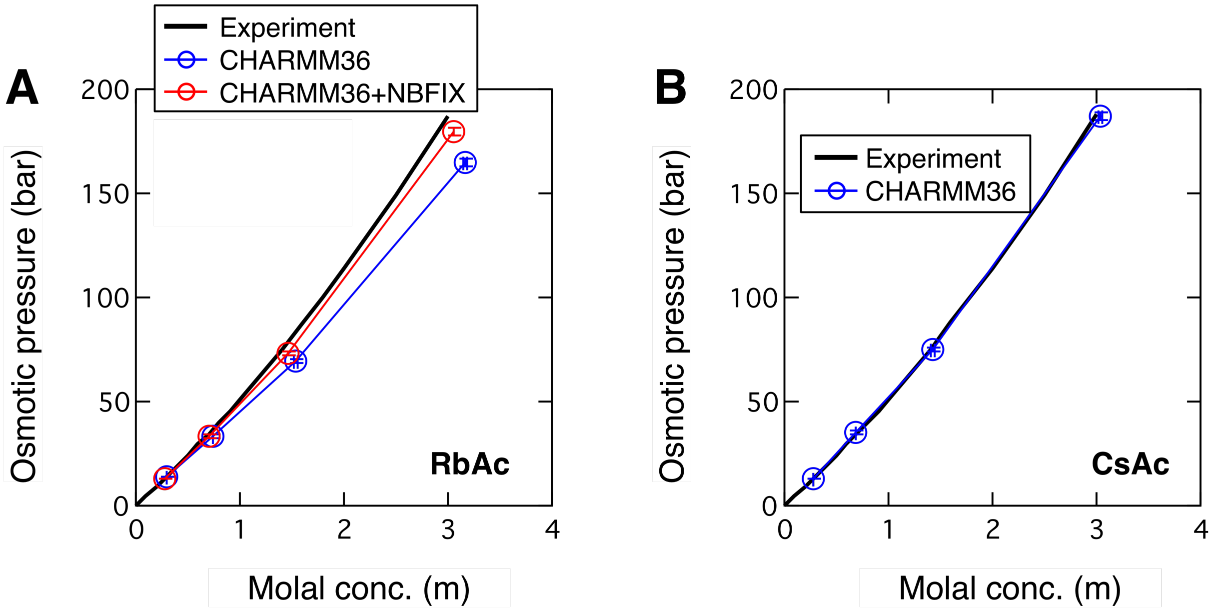

Figure S7: Validation and calibration of Rb^{+}–Ac^{-} (A) and Cs^{+}–Ac^{-} (B) ion pair interactions for the CHARMM36 force field using osmotic pressure simulations. The simulation method for computing osmotic pressure was similar to that used in Ref. 2 and 3. NBFIX corrections, if necessary, were applied to the Lennard-Jones R_{min} parameters for cation–acetate oxygen atom pairs. Experimental data were taken from Ref. 4. See Table 4 for the changes in R_{min} parameters.

References

(1) Joung, I. S.; Cheatham, T. E. Determination of Alkali and Halide Monovalent Ion Parameters for Use in Explicitly Solvated Biomolecular Simulations. *J. Phys. Chem. B* **2008**, *112*, 9020–9041.

(2) Yoo, J.; Aksimentiev, A. Improved Parametrization of Li^+, Na^+, K^+, and Mg^{2+} Ions for All-Atom Molecular Dynamics Simulations of Nucleic Acid Systems. *J. Phys. Chem. Lett.* **2012**, *3*, 45–50.

(3) Yoo, J.; Aksimentiev, A. Improved Parameterization of Amine–Carboxylate and Amine–Phosphate Interactions for Molecular Dynamics Simulations Using the CHARMM and AMBER Force Fields. *J. Chem. Theory Comput.* **2016**, *12*, 430–443.

(4) Robinson, R. A.; Stokes, R. H. *Electrolyte Solutions*; Butterworths scientific publications, 1959.

(5) Hart, K.; Foloppe, N.; Baker, C. M.; Denning, E. J.; Nilsson, L.; MacKerell, Jr., A. D. Optimization of the CHARMM Additive Force Field for DNA: Improved Treatment of the BI/BII Conformational Equilibrium. *J. Chem. Theory Comput.* **2012**, *8*, 348–362.