

The correlation between micelle morphology of surface-active ionic liquids with self-assembly and thermodynamic characteristics: coarse-grained MD simulation and experiment

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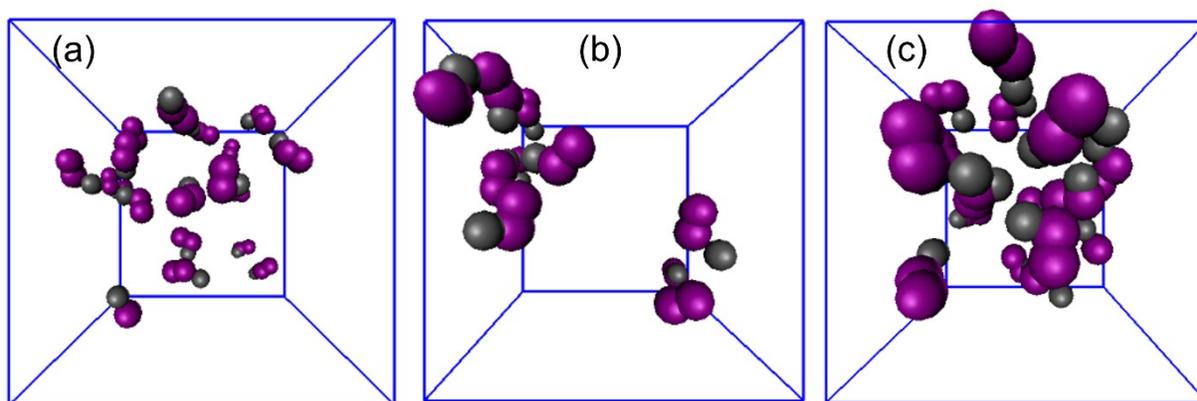


Figure S1. Final snapshots of BMI at different concentration: (a) before the CMC point, (b) at the CMC point, and (c) after the CMC point. Head and tail groups are shown in purple and grey colors, respectively.

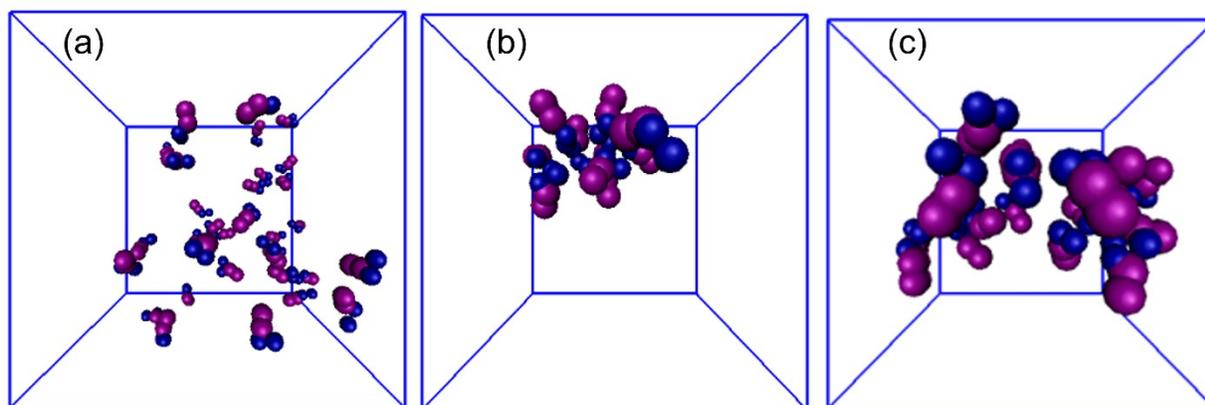


Figure S2. Final snapshots of HMI at different concentration: (a) before the CMC point, (b) at the CMC point, and (c) after the CMC point. Head and tail groups are shown in purple and blue colors, respectively.

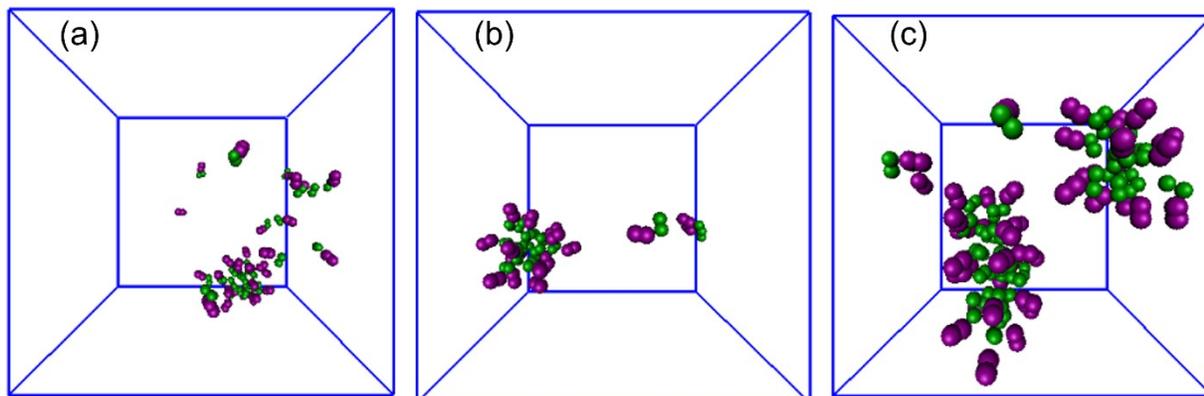


Figure S3. Final snapshots of OMI at different concentration: (a) before the CMC point, (b) at the CMC point, and (c) after the CMC point. Head and tail groups are shown in purple and green colors, respectively.

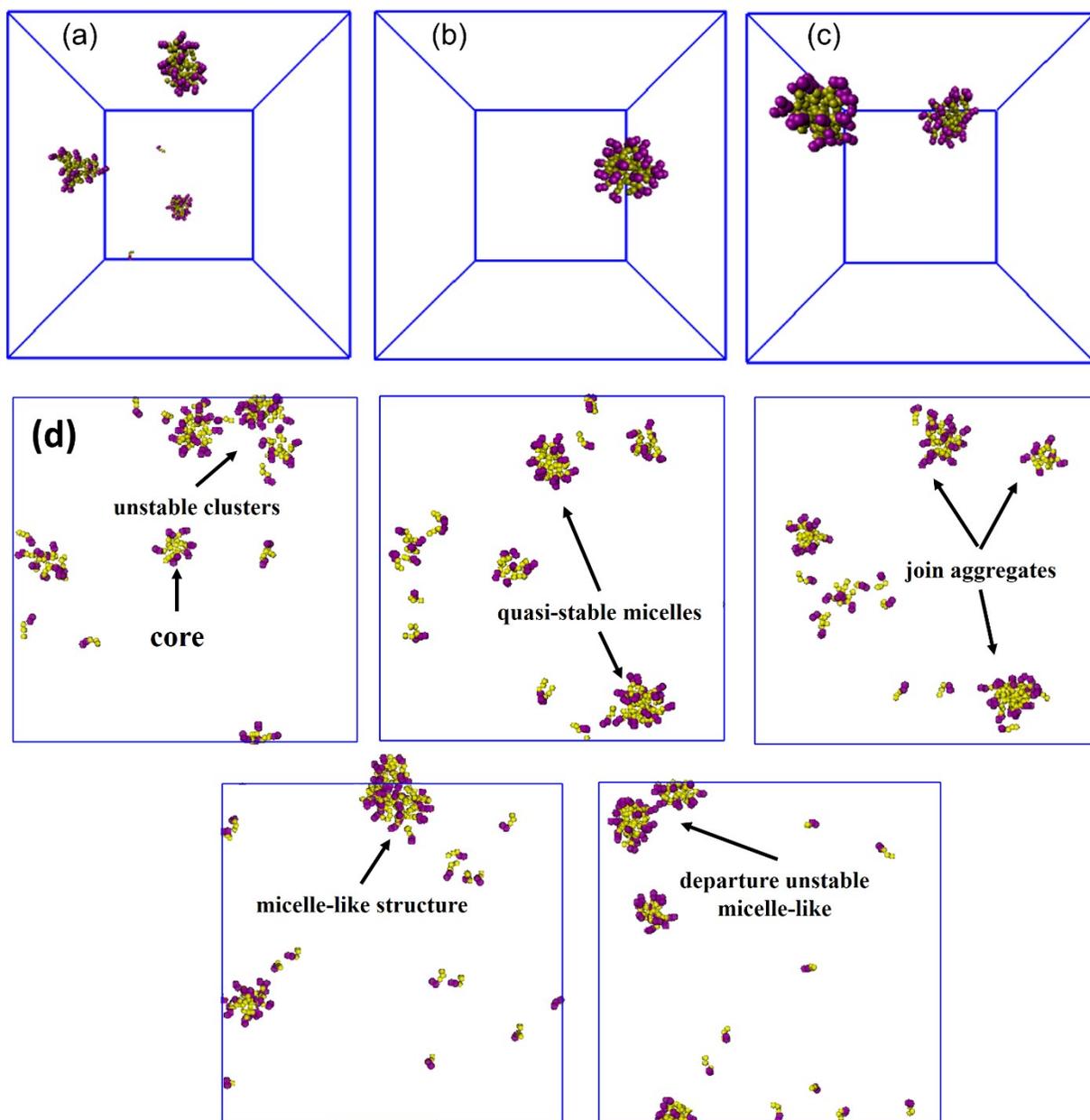


Figure S4. Final snapshots of DMI at different concentration: (a) before the CMC point, (b) at the CMC point, and (c) after the CMC point. Head and tail groups are shown in purple and yellow colors, respectively. (d) The process of aggregation of DMI below CMC. different sizes and numbers of quasi-stable clusters before CMC, which can act as nuclei in solution for higher-order aggregation.

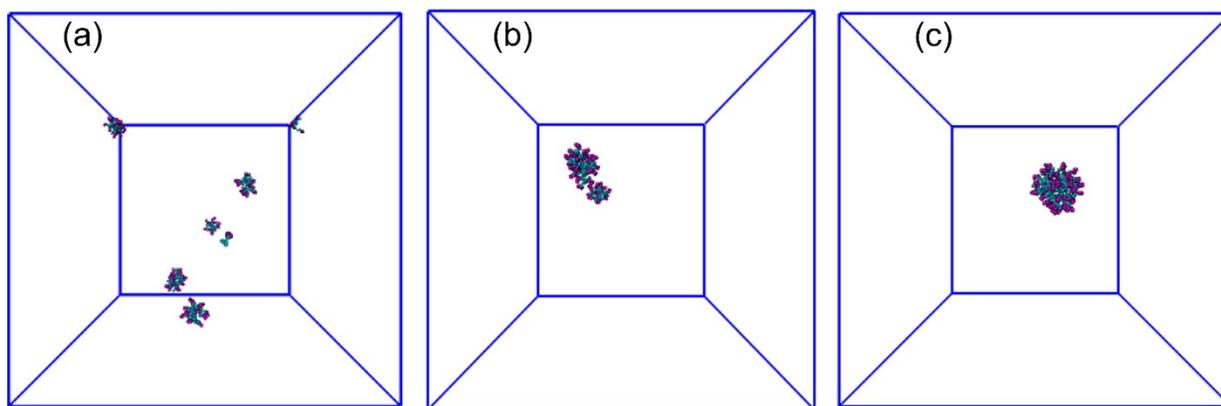


Figure S5. Final snapshots of DOMI at different concentration: (a) before the CMC point, (b) at the CMC point, and (c) after the CMC point. Head and tail groups are shown in purple and cyan colors, respectively.

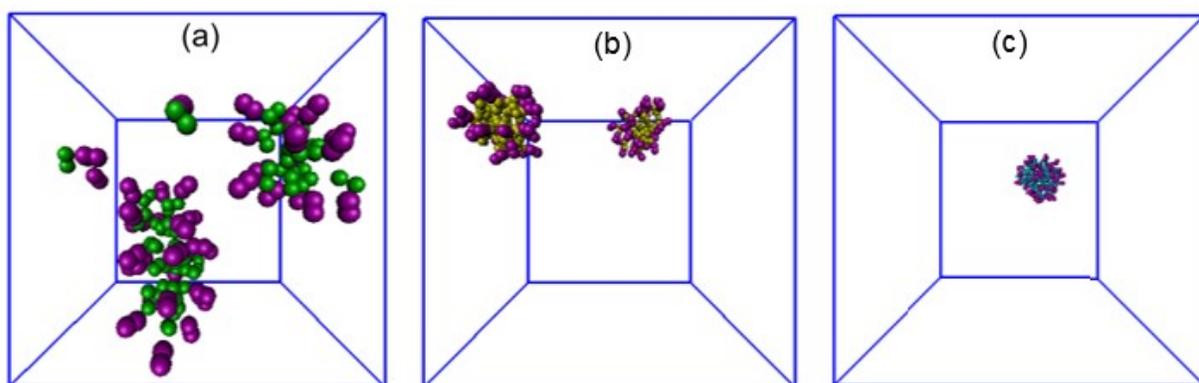


Figure S6. Final snapshots after the CMC : (a) OMI, (b) DMI, (c) DOMI. Head and groups are shown in purple and tail groups are shown in green, yellow and cyan colors, respectively.

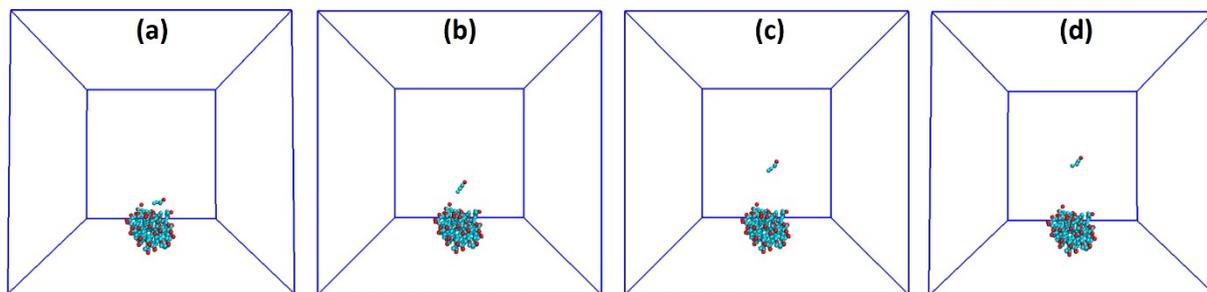


Figure S7. Final snapshots of umbrella simulations : (a) 0.20 nm, (b) 0.40 nm, (c) 0.70 and (d) 0.90 nm. Head groups are shown in red and tail groups are colored by cyan.