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Continuum-based coarse-grained water potentials for structural prediction in confined environments¹ S.Y. MASHAYAK, N.R. ALURU, Department of Mechanical Science and Engineering, Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign — We develop the single site coarse-grained (CG) potential for structural prediction of the confined water. CG potentials allow computationally efficient simulations, which can access larger time- and length-scales compared to fully atomistic simulations. In the literature, various CG techniques have been used to develop CG potentials for structural prediction of bulk water. Due to the inherent inhomogeneity of the confined water system and water's ability to form directional hydrogen-bonds, development of CG potentials for confined water is a formidable task, and not much progress has been done to solve this problem. Herein, we systematically derive the single site CG potentials for the confined water, and show that these potentials can be used in the multi-scale quasi-continuum framework as well as in the CG molecular dynamics (MD) simulations to predict, in a computationally efficient manner, the atomic-level structure of the water confined in two types channels- a silicon slit channel and a graphite slit channel. Our results show that the center of mass density profiles of the water predicted by the CG model are in good agreement with all-atom MD results across multiple length scales, i. e., from few atomic diameters channel widths to 100s of nm.

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