Abstract Submitted
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Nucleationand surface induced crystallization in supercooled liquid water[1] GIOVANNA RUSSO, Department of Material and Chemical Engineering, Politecnico di Torino,ITALY and Department of Chemistry, University of California, Davis, CA 95616 , TIANSHU LI, DAVIDE DONADIO, Department of Physics, University of California, Davis, CA 95616, GIULIA GALLI, Department of Chemistry and Department of Physics, University of California, Davis, CA 95616 — Understanding crystallization of water into ice is a very challenging problem, both experimentally and theoretically; in particular, the spatial and temporal resolutions required to characterize the crystallization process at the atomic scale are not yet accessible to experiment. Here we employ a combination of molecular dynamics simulations and advanced sampling techniques to study nucleation in supercooled liquid water. Recently, such an approach has been successfully applied to study nucleation in supercooled liquid silicon [1,2]. The results of our simulations, carried out using a coarse grain potential [3], are used to analyze nucleation rates at various temperatures and to investigate the role played by the presence of surfaces in the freezing processes.

[1] T. Li, D. Donadio and G. Galli, Nat. Mat. 9, 726730 (2009)
[2] T. Li, D. Donadio and G. Galli, J. Chem. Phys., in press
[3] V. Molinero and E. B. Moore J. Phys. Chem. B 113, 40084016 (2009)

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