Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Diffusion of Water Nanodroplets on MoS_2 Monolayer[1] BEIBEI WANG, CACS, Dept. of Physics Astronomy, University of Southern California, RAJIV KALIA, PRIYA VASHISHTA, AIICHIRO NAKANO, CACS, Dept. of Physics Astronomy, Dept. of Chemical Engineering Materials Science, Dept. of Computer Science, University of Southern California — Diffusion of water (H_2O) on the molybdenum disulfide (MoS_2) surface has recently attracted a great deal of attention. We have performed molecular dynamics (MD) simulation to study the diffusion of water nanodroplets on a monolayer of MoS_2. Our simulation reveals that water nanodroplets diffuse rapidly on the MoS_2 monolayer and the diffusion coefficient is inversely proportional to the nanodroplet radius. We also find that the H_2O molecular distribution at the H_2O-MoS_2 interface is akin to the MoS_2 layered structure and that friction coefficients of nanodroplets are small at the MoS_2 surface.

[1]This work was supported as part of the Computational Materials Sciences Program funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

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Date submitted: 11 Nov 2016 Electronic form version 1.4