Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

The thickness dependence of surface energy and contact angle of water on ultrathin MoS_2 film[1] YANHUA GUO, College of Materials Science and Engineering, Nanjing Tech University; Department of Materials Science and Engineering, University of Utah, FENG LIU, Department of Materials Science and Engineering, University of Utah — The properties of ultrathin 2D materials generally show a strong thickness dependence. Using first-principles methods, we have systematically calculated surface energy and surface stress of MoS_2 films as a function of thickness from one to 12 layers, using two van der Waals functional based approaches (vdW-DF and DFT-D2). Based on the calculated surface energies, which increases with the increasing thickness, we further analyze the surface contact angle of water droplet on MoS_2 film surface using Young's equation as a function of thickness, in comparison with experiments, from which the water-MoS_2 interfacial energy and its MoS_2 thickness dependence is derived. These results will be useful for future studies of physical and chemical properties of ultrathin MoS_2 films.

[1]This work is supported by China Scholarship Council (Grant No. 201408320015) and DOE-BES (Grant No. DEFG02-04ER46148).

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Date submitted: 14 Nov 2014 Electronic form version 1.4