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Consistent picture for the wetting structure of water/Ru(0001)
SHENG MENG, Department of Applied Physics, Chalmers University of Technology and Gothenburg University, SE-412 96 Gothenburg, Sweden, E.G. WANG, Institute of Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing, 100080, PR China, CHRISTIAN FRISCHKORN, MARTIN WOLF, Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany, SHIWU GAO, Department of Applied Physics, Chalmers University of Technology and Gothenburg University, SE-412 96 Gothenburg, Sweden — The wetting layer of D2O on Ru(0001) has been reanalyzed with ab-initio molecular dynamics and full-potential calculation. Comparison of vibrational spectra and work function with experiments favors the picture of molecular wetting rather than partial dissociation. A mixture structure consisting of both hydrogen-up and hydrogen-down bilayers is found to be consistent with experiments. The barrier and minimum energy path for bilayer dissociation have been determined. The dissociation barrier is larger than that for desorption, suggesting that dissociation is kinetically forbidden at low temperatures. These finding resolve the current controversy between previous calculations and experimental observations.

Shiwu Gao
Department of Applied Physics, Chalmers University of Technology
and Gothenburg University, SE-412 96 Gothenburg, Sweden

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