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Stabilization of the O p2x2 phase on Cu(001) sheltered by wrinkled BN over-layer¹ YONG-SUNG KIM, Korea Research Institute of Standards and Science, Yuseong, Daejeon 305-340, Korea, CHUANXU MA, AN-PING LI, MINA YOON, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA — The $2\sqrt{3}\times\sqrt{3}R45$ phase of oxygen (O) on the Cu(001) surface has been observed in scanning tunneling microscopy (STM) measurements. Although the p2x2 phase of O on the Cu(001) surface has been proposed theoretically to be the most stable in O-lean conditions, it has not been observed in experiments for a long time. Recently, the O p2x2 phase has been found in STM on the Cu(001) surface with an overlying BN monolayer. In this theoretical study, we investigate what the role of BN over-layer is to stabilize the O p2x2 phase on the Cu(001) surface. The BN over-layer is lattice-matched with the Cu(001) surface and the BN mono-layer sheet is periodically wrinkled along the BN arm-chair direction and along the [100] or [010] direction on the Cu(001) surface. The inter-layer space between the Cu(001) surface and the bulge of the wrinkled BN sheet is found to play as a preferential shelter for O to be adsorbed, and the boundary of the BN inner wall along the [010] or [100] direction makes the p2x2 phase more favorable against the 45-tilted $2\sqrt{3}\times\sqrt{3}R45$ phase of O on the Cu(001) surface.

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Yong-Sung Kim
Korea Research Institute of Standards and Science, Yuseong, Daejeon 305-340, Korea

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