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Two-dimensional square structures of CuO and Cu2O monolayer.[1] YUYANG ZHANG, Vanderbilt Univ; Oak Ridge National Lab, KUIBO YIN, YILONG ZHOU, LITAO SUN, Southeast University, MATTHEW F. CHISHOLM, Oak Ridge National Lab, SOKRATES T. PANTELIDES, Vanderbilt Univ; Oak Ridge National Lab, WU ZHOU, Oak Ridge National Lab — Among 2D crystals, monolayer (ML) oxides are interesting because of the coupling of quantum confinement to other degrees of freedom that are present in bulk materials. However, as most oxides are not layered structures, fabrication of 2D oxides has been limited. Current studies focus on either two-to-three atomic layers thick materials, such as the exfoliated perovskites, or supported films that are bonded to the substrate. Unsupported single-atom-thick oxides have not been reported. Here we report the fabrication of single-atom-thick copper oxide ML. Quantum mechanical calculations indicate that free-standing copper oxide MLs are stable wide-bandgap semiconductors with a variable chemical stoichiometry ranging from CuO to Cu2O at similar lattice constants. The stoichiometry variation changes the bandgap from indirect for CuO ML to direct for Cu2O ML, suggesting that the electronic and optical properties of ML copper oxides can be tuned by the oxygen content.

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