

Abstract Submitted
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Observation of charge redistribution during bond formation in one-dimensional alkali-metal wires GUIDO FRATESI, Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, 20125, Italy, CONGCONG HUANG, Stanford Synchrotron Radiation Laboratory, Menlo Park, California 94025, USA, DONALD A. MACLAREN, Dept. of Physics, University of Glasgow, Glasgow G12 8QQ, UK, WEIDONG LUO, Materials Sci. and Technology Div., Oak Ridge National laboratory, Tennessee 37831, USA, WILLIAM ALLISON, Cavendish Laboratory, University of Cambridge, CB3 0HE, UK, GIAN PAOLO BRIVIO, Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, 20125, Italy — We have tracked the formation of Li wires in the Li/Cu(100) system. Wire formation is driven by the increased in-plane adatom density as Li coverage increases from 0.5 to 0.6 Monolayers (ML). We used a combination of Helium Atom Scattering (HAS) and Density Functional Theory (DFT) to show the emergence of anisotropic, 1-dimensional inter-Li bonding. HAS, which is sensitive to the outermost electronic charge density, shows a transition to an unexpectedly large, 1-dimensional electronic corrugation at a coverage of 0.6ML. DFT calculations identify the corrugation as the formation of a corrugated array of Li wires. Bond formation along the Li wires is enabled by charge donation from the substrate but without significant change to the layer spacing.

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