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Kinetic pathway for the formation of Fe nanowires on stepped Cu(111) surfaces YINA MO, Physics Department, Harvard University, KALMAN VARGA, Physics Department, University of Tennessee; Condensed Matter Science Division, Oak Ridge National Lab, EFTHIMIOS KAXIRAS, Physics Department and Division of Engineering and Applied Sciences, Harvard University, ZHENYU ZHANG, Condensed Matter Science Division, Oak Ridge National Lab; Physics Department, University of Tennessee — We report the discovery of a novel kinetic pathway for the formation of one-dimensional Fe nanowires of single atom width on stepped Cu(111) surfaces. This pathway, identified through extensive total-energy calculations within density functional theory, establishes that the stable structure involves a row of Fe atoms in the upper edge of a step. The formation of the surface wire is preceded by facile incorporation of an initial row of Fe atoms into the surface layer at one lattice constant away from the step edge, which then acts as an attractor for the second, exposed row of atoms. Under this new frame of wire structure, magnetic properties of these wires are studied.

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