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Structure of self-assembled Mn atom chains on Si(001) RENAN VILLARREAL, MARIA LONGOBARDI, SIGRUN A. KOESTER, Department of Quantum Matter Physics, University of Geneva, Geneva, CH-1211, Switzerland, CHRISTOPHER J. KIRKHAM, Division of Precision Science and Technology and Applied Physics, Graduate School of Engineering, Osaka University, 2-1, Yamada-oka, Suita, Japan, DAVID BOWLER, London Centre for Nanotechnology and Department of Physics and Astronomy, University College London, London WC1E 6BT, United Kingdom, CHRISTOPH RENNER, Department of Quantum Matter Physics, University of Geneva, Geneva, CH-1211, Switzerland — Mn has been found to self-assemble into atomic chains running perpendicular to the surface dimer reconstruction on Si(001). They differ from other atomic chains by a striking asymmetric appearance in filled state scanning tunneling microscopy (STM) images. This has prompted complicated structural models involving up to three Mn atoms per chain unit. Combining STM, atomic force microscopy and density functional theory we find that a simple necklace-like chain of single Mn atoms reproduces all their prominent features, including their asymmetry not captured by current models. The upshot is a remarkably simpler structure for modelling the electronic and magnetic properties of Mn atom chains on Si(001).

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