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LEED Study of the Structure of $Si(111) - (2\sqrt{3} \times 2\sqrt{3}) R30^{\circ} - 4B +$ 14Sn Phase YING-TZU HUANG, RENEE DIEHL, Department of Physics, Penn State University, WEISONG TU, DANIEL MULUGETA, Department of Physics and Astronomy, University of Tennessee, PAUL SNIJDERS, PAUL KENT, Oak Ridge National Laboratory, HANNO WEITERING, Department of Physics and Astronomy, University of Tennessee — While doping of bulk materials to control their properties has been hugely successful, doping of inherently low-dimensional surface-based electronic structures remains a challenge: dopant atoms not only affect the electronic carrier density but also significantly disrupt the surface atomic structure, and often lead to localized changes of atomic and electronic properties. We developed a modulation doping approach to dope surface structures with the dopants that are located below the surface of a two-layer thick Sn film on Si(111). The doped Sn film exhibits a temperature dependent structural and electronic phase transition that is absent in the undoped structure. In this study, we have used lowenergy electron diffraction (LEED) to determine the surface structure. The LEED experiment was performed at 90 K. The energy range was 40-500 eV, for a total of 7126eV from 20 independent beams. The structure models considered include those based on the scanning tunneling microscopy (STM) images and density functional theory (DFT) calculations. The best agreement obtained was proposed in a recent DFT study produces a Pendry R-factor of 0.36. However, the level of agreement is not yet convincing and many more structure models are being tested.

> Ying-Tzu Huang Department of Physics, Penn State University

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