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**Temperature Dependent Phases of Sr on Si (001): First principles theory and experiment** KEVIN F. GARRITY, MYRTLE-ROSE PADMORE, YARON SEGAL, JAMES W. REINER, FRED J. WALKER, CHARLES H. AHN, SOHRAB ISMAIL-BEIGI, Yale University — Understanding and predicting temperature dependent surface phases from first principles can be invaluable in developing and optimizing processes for the growth of epitaxial structures. In particular, an ordered sub-monolayer phase of Sr on Si (001) plays a key role in determining the quality of the interface in the most commonly used method for growing epitaxial oxides on Si. Using density functional theory, we build a first principles model of sub-monolayer Sr on Si, which we use to determine the temperature dependent phase equilibrium between an ordered 1/6 ML structure and a disordered lattice gas. In addition, we experimentally determine this phase diagram using RHEED and find quantitative agreement between theoretical predictions and experiment.

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