

Abstract Submitted  
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**Empirical modeling of STM imaging and tunneling spectroscopy of adsorbates on the Si(111)7x7 surface.**<sup>1</sup> WEIMING LIU, Department of Physics, University of Lethbridge, Lethbridge, Alberta, T1K 3M4, Canada, STEVEN A. HORN, Department of Physics, University of Lethbridge, Lethbridge, Alberta, T1K 3M4, Canada, POUYA MARAGHECHI, Department of Physics, University of Lethbridge, Lethbridge, Alberta, T1K 3M4, Canada, S.N. PATITSAS, Department of Physics, University of Lethbridge, Lethbridge, Alberta, T1K 3M4, Canada — To accurately simulate experimentally measured STM results have developed an atomic orbital model for the top layer atoms of the Si(111)7x7 surface. Adatom, restatom and corner hole dangling bonds are represented by  $sp^3$  hybrids of hydrogen-like orbitals adjusted to have the correct work function and including tip-induced electric field effects. Peak energies, widths and other DOS information, were extracted from known experimental data and theoretical calculations.<sup>1</sup> Restatom and adatom charge transfer was included. Back-bonding orbitals for adatoms, restatoms and dimers were also used. Bulk DOS data was used for deeper bonding orbitals. The Tersoff-Hamann approach is used calculate the tunneling current.<sup>2</sup> We will present numerically calculated topographic images as well as spectra and compare to experiments. [1]Brommer *etal*, *Surf. Sci.* **314**, 57 (1994). [2]Tersoff and Hamann, *Phys. Rev. B*, **31**, 805 (1985).

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Steve Patitsas  
Department of Physics, University of Lethbridge, Lethbridge, Alberta, T1K 3M4, Canada

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