

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Theoretical Study of tip apex electronic structure in Scanning Tunneling Microscope¹ HEESUNG CHOI, MIN HUANG, Department of Materials Science & Engineering and Department of Physics, The University of Texas at Dallas, JOHN RANDALL, Zyvex Lab, KYEONGJAE CHO, Department of Materials Science & Engineering and Department of Physics, The University of Texas at Dallas — Scanning Tunneling Microscope (STM) has been widely used to explore diverse surface properties with an atomic resolution, and STM tip has played a critical role in controlling surface structures. However, detailed information of atomic and electronic structure of STM tip and the fundamental understanding of STM images are still incomplete. Therefore, it is important to develop a comprehensive understanding of the electronic structure of STM tip. We have studied the atomic and electronic structures of STM tip with various transition metals (TMs) by DFT method. The d-electrons of TM tip apex atoms show different orbital states near the Fermi level. We will present comprehensive data of STM tips from our DFT calculation. Verified quantification of the tip electronic structures will lead to fundamental understanding of STM tip structure-property relationship. This work is supported by the DARPA TBN Program and the Texas ETF.

¹DARPA Tip Based Nanofabrication Program and the Emerging Technology Fund of the State of Texas

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Date submitted: 27 Nov 2010

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