Possibility of Imaging Lateral Profiles of Tetrahedral Hybrid Orbitals in Real Space with NC-AFM

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The concept of tetrahedral hybrid orbital was introduced by Pauling and Slater [1] in 1929 as the bonding mechanism of crystalline Si, Ge, most carbon compounds as the basis of life, and diamond. To date, those sp^3 orbitals have been only in theorist's mind, never perceived directly. Using perturbation theory [2] and standard atomic orbital data [3], we show that with NC-AFM [4], it is possible to resolve the lateral profile of sp^3 orbitals in real space.

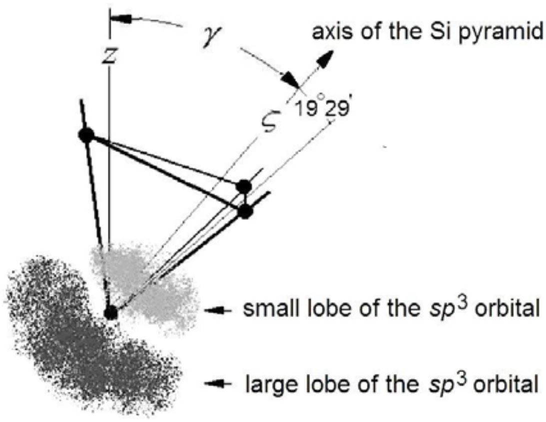

Figure 1: A Si cluster picked up by a tip. The orientation of the apex axis with the z-axis is random. The maximum value of angle γ is 71˚. There is a 20% chance for $\gamma > 60˚$.

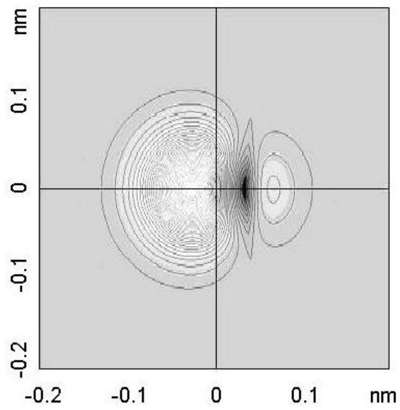

Figure 2: The predicted force distribution. The grey background represents zero force. White represents attractive force and black represents repulsive force. Angle γ is 65˚.

The experimental condition is to use Si(111)7×7 as the sample. Initially, the tip can be W, Pt-Ir, or silicon. By gently touching the sample, the tip can pick up a Si cluster. The orientation of the Si cluster with regard to *z*-axis is random. See Figure 1. There is a 20% chance the angle γ is greater than 60˚. Then, the small lobe of the sp^3 orbital is exposed to the *z*-plane. With the sp^3 dangling bonds on the Si(111)7×7 as the probe, both lobes of the sp^3 orbital can be imaged. Each image of the sp^3 dangling bond is split into a large, half-moon shaped feature and a small feature. Although both STM and AFM can be used, AFM has the advantage that between the two lobes, there is a **repulsive force** region**,** whereas with STM, the tunnelling conductance would hardly be zero. Therefore the contrast with AFM is higher, see Figure 2.

[1] L. Pauling, J. Amer. Chem. Soc., 53, 1367 (1931).
[2] C. Julian Chen, *Introduction to Scanning Tunneling Microscopy* (1993).
[3] E. Clementi and P. Roetti, Atom Data and Nuclear Data Tables, 14, 429 (1974).
[4] S. Morita, R. Wiesendanger, and E. Meyer, Eds. *Noncontact Atomic Force Microscopy*, Springer 2002.