

**Hou *et al.* Reply:** Pascual *et al.* [1] have performed independent scanning tunneling microscopy (STM) experiments on  $C_{60}$  molecules adsorbed on Si(111)-(7  $\times$  7) and have obtained results which coincide, in many respects, with those in our recent publication [2]. They disagree with us, however, on whether the STM images depend on the bias voltages. By noting that the calculated local densities of states (LDOS) of the  $C_{60}$  highest occupied molecule orbitals (HOMO) agree well with both their positive and negative bias images, they conclude that the STM images do not depend on the bias voltages (see Fig. 1 of Pascual *et al.* [1]). Since the positive bias images are supposed to agree with LDOS of the lowest unoccupied molecular orbitals (LUMO), they thus question the applicability of the Tersoff-Hamann (TH) theory [3] in such a system.

We only need to point out that the TH theory says nothing about whether or not a specific system could exhibit some visual similarity between its LDOS of HOMO and that of LUMO. In fact, Fig. 1a is the calculated LDOS for the LUMO of an isolated  $C_{60}$  molecule with the pentagon facing the substrate, and it matches equally well, if not better, with Figs. 1a and 1c of Pascual *et al.*, compared with their Figs. 1g and 1e. (Note that their Fig. 1a is a double  $C_{60}$  image and there is a bright pentagon centered on each  $C_{60}$ ). Thus, there is no reason not to assign their observed positive bias STM images to the LUMO images, and the negative bias STM images to the HOMO images as implied in the TH theory.

On contrary to the claim of Pascual *et al.* [1], their STM images are fully in agreement with our results and analysis. It is encouraging to see that their negative bias images (Figs. 1b and 1d) reveal more detailed information than the stripe structure of our Figs. 2a1 and 2b1 in Ref. [2]. This information could be used to explore the splitting of the  $C_{60}$ 's HOMO, if a series of images is recorded with the change of the bias voltage.

While a more sophisticated theoretical calculation is always desirable, evidence shows that the TH theory is adequate for identifying, from the STM images, the molecular orientations of  $C_{60}$  adsorbed on Si(111)-(7  $\times$  7) surfaces, as we have demonstrated.

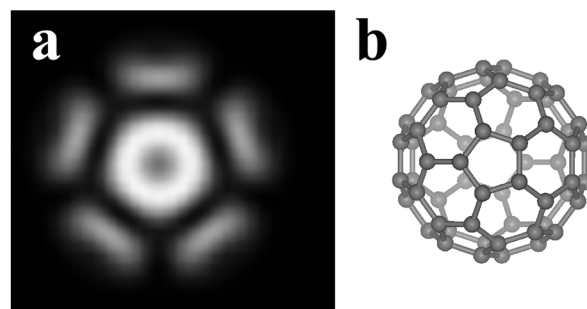


FIG. 1. (a) Simulated LDOS for the LUMO of an isolated  $C_{60}$  molecule with the pentagon facing the substrate. STM tip scanning height is 16 bohr; (b) top view of the  $C_{60}$  molecule with the pentagon facing the substrate.

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