Artificial two-dimensional Mott insulating superstructures with a large Mott gap: Theoretical Formalism

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To have a better understading of the experimental observations, we construct single-band Hubbard model with renormalized hopping coefficients to describe these systems and calculate the local density of states by using cluster perturbation theory (CPT) [1, 2].

For the $(3\sqrt{7} \times 3\sqrt{7})R19.1^\circ$ surface (referred to as Phase 1 in the followings), the corresponding proposed atomic structural is shown in Fig. 1(g). The unit cell contains twenty-three sites while three of them are somewhat isolated, see the three blue circles in Fig. 1(d). Considering that the hopping amplitude is inversely proportional to the square of the distance, it is reasonable to neglect the three isolated sites in a simplified model. We only include these hopping terms shown in Fig. 2 and the resulting Hamiltonian takes the following form:

$$H = \sum_{<i,j>\sigma} t_{ij}(c^\dagger_{i\sigma}c_{j\sigma} + \text{H.c.}) + U\sum_i n_{i\uparrow}n_{i\downarrow} \quad (1)$$

where t_{ij} is the effective hopping amplitude and U the effective on-site Coulomb repulsion. Here, we take $t_{ij} = -1/r^2_{ij}$, where r_{ij} is the distance between i-th site and j-site. See appendix for the coordinates of these sites shown in Fig. 2.

For this model Hamiltonian, we first consider the non-interacting case (*i.e.*, $U = 0$). The corresponding energy band and local density of states are shown in Fig.

[1] C. Gros and R. Valentí, Phys. Rev. B **48**, 418 (1993).
[2] D. Sénéchal, D. Perez, and M. Pioro-Ladrière, Phys. Rev. Lett. **84**, 522 (2000).

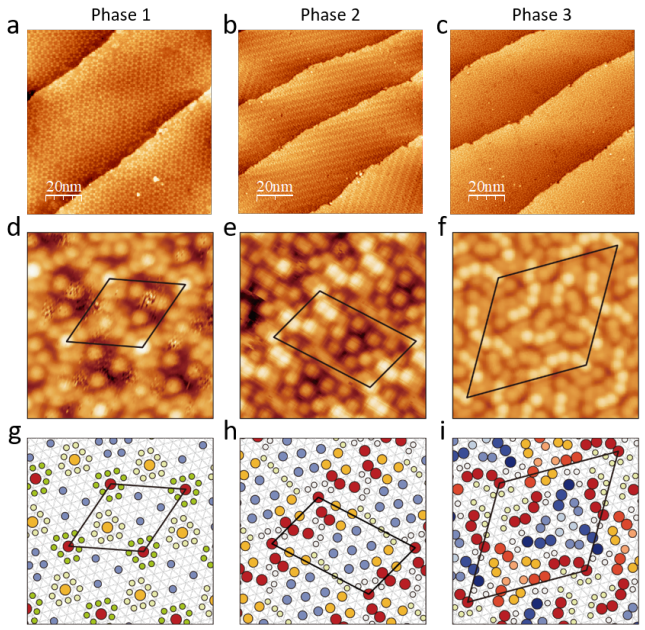

FIG. 1. (Color online) STM characterization of three new superstructures of Sn sub-monolayers on Si(111). (a)-(c) Large-scale STM image (size: 100×100 nm^2) taken on $(3\sqrt{7} \times 3\sqrt{7})R19.1°$, $(\sqrt{133} \times 4\sqrt{3})$ and (13×13) surfaces. They are taken at $U = +3.5V$, $U = -2V$ and $U = -2V$ ($I_t = 100pA$) respectively. (d)-(f) The atomically resolved STM images of them taken at $U = -2V, I_t = 200pA$. The surface unit cells of them are marked in black. (g)-(i) The corresponding proposed atomic structural models. The marked surface unit cells in (g)-(i) are the same as these in (d)-(f).

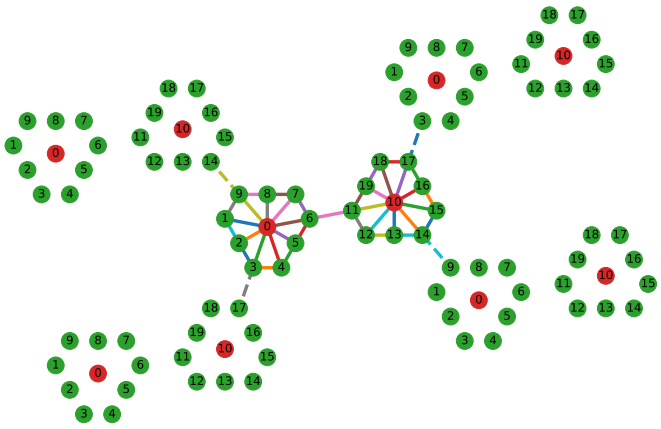

FIG. 2. (Color online) Demonstration of the hopping terms for Phase 1. The unit cell has twenty sites labeled from 0 to 19. The soild and dashed lines correspond to the hopping terms $t_{ij}(c^\dagger_{i\sigma}c_{j\sigma} + \text{H.c.})$, where $t_{ij} = -1/r^2_{ij}$ and r_{ij} is the distance from i-th to j-th site.