# Theoretical Formalism

(Dated: December 10, 2020)

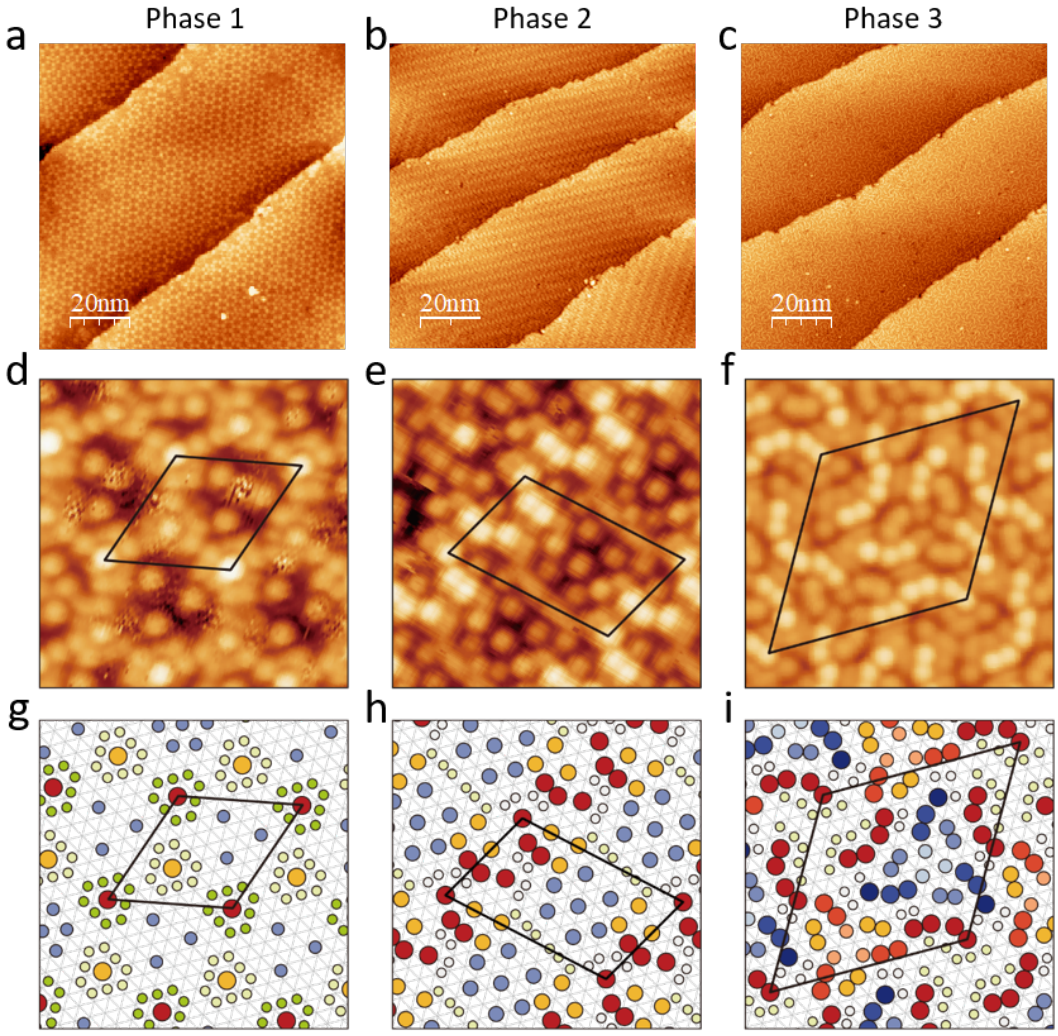


FIG. 1. (Color online) STM characterization of three new superstructures of Sn sub-monolayers on Si(111). (a)-(c) Large-scale STM image (size: 100 × 100 nm$^2$) taken on $(3\sqrt{7}\times 3\sqrt{7})R19.1^\circ$, $(\sqrt{133}\times 4\sqrt{3})$ and $(13\times 13)$ surfaces. They are taken at $U=+3.5V$, $U=-2V$ 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).

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].

To have a better understanding of the experimental observations, we adopt the single-band Hubbard model with modulated hopping coefficients and use cluster perturbation theory (CPT)[1, 2] to calculate the spectral function as well as density of states of the model Hamiltonians. For the $(3\sqrt{7}\times 3\sqrt{7})R19.1^\circ$ surface (referred to as Phase 1 in the following), the STM topographic image are shown in Fig. 1(a) and Fig. 1(d). Based on the proposed atomic structural shown in Fig. 1(g), we constructed a single-band Hubbard model with modulated hopping coefficients to describe the system. The model Hamiltonian takes the following form:

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

[1] C. Gros and R. Valentí, Phys. Rev. B **48**, 418 (1993).

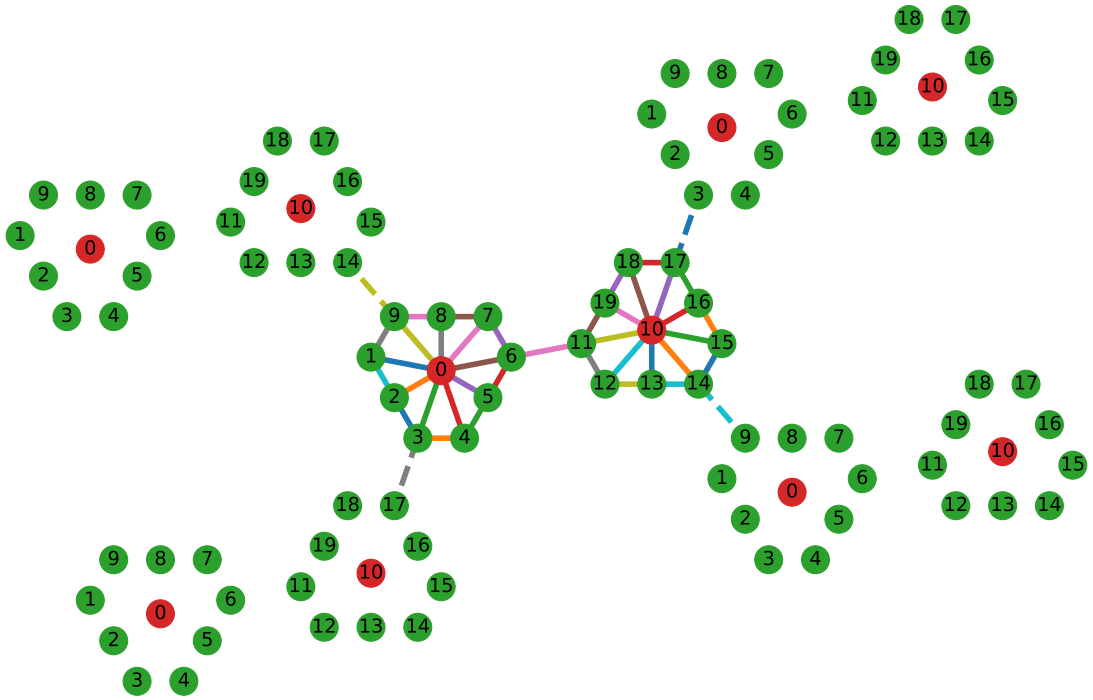


FIG. 2. (Color online) Demonstration of the hopping terms for Phase 1. The unit cell has twenty sites labeled from 0 to 19. The soild and dashed lines correspond to the hopping terms $t_{ij}(c^{\dagger}_{i\sigma}c_{j\sigma} + \text{H.c.})$, where $t_{ij} = -1/r^2_{ij}$ and $r_{ij}$ is the distance from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

[2] D. Sénéchal, D. Perez, and M. Pioro-Ladrière, Phys. Rev. Lett. **84**, 522 (2000).