Supplemental Material for

Energetics and kinetics of Cu atoms and clusters on Si(111)-7×7 surface: first-principles calculations

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This file includes:

S1. The top and side views of the whole slab dimer-adatom-stacking-fault (DAS) model.

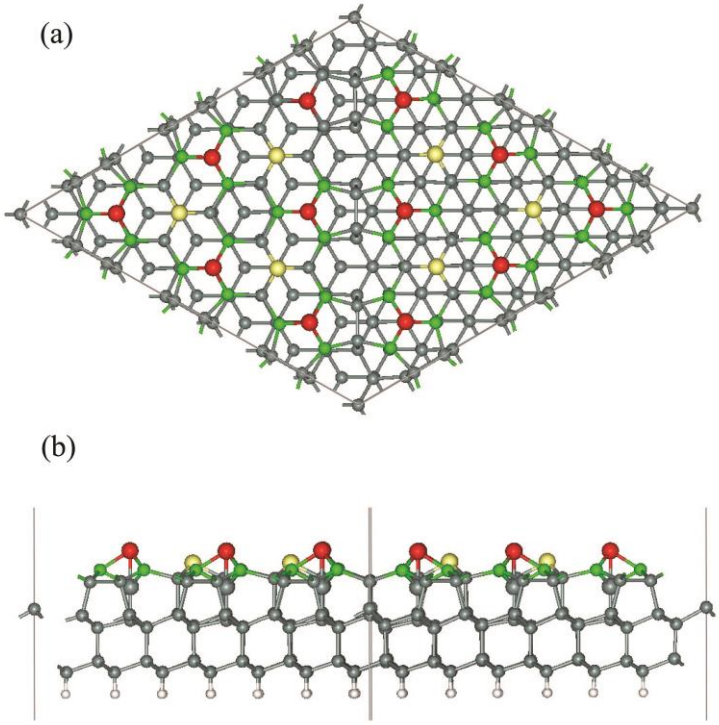

Figure 1S: The top **(a)** and the side **(b)** views of the whole slab dimer-adatom-stacking-fault (DAS) model. Red, yellow, green, gray and white balls represent the Si adatoms, Si rest atoms, Si backbond atoms, Si bulk atoms and H atoms, respectively.

S2. Simulated STM image of the most stable Cu_6/Si(111)-(7×7) complex versus the experimental STM pattern of Cu cluster arrays on Si(111)-(7×7) with a coverage around 0.15 ML.

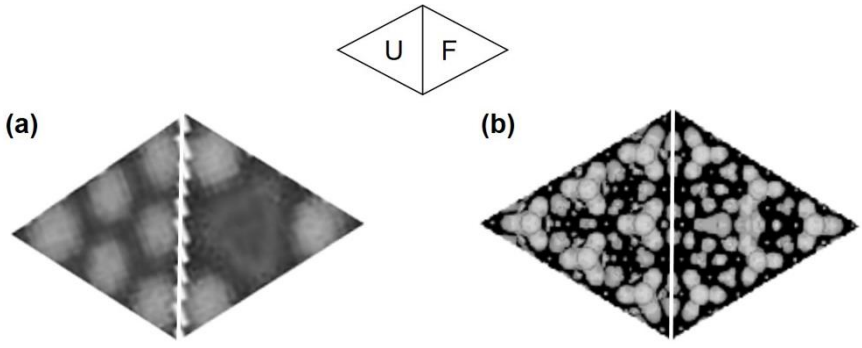

Figure 2S: (a) Experimental STM image of Cu cluster arrays on Si(111)-(7×7) with a coverage around 0.15 ML (see Ref. 13); (b) Simulated STM image of the most stable Cu_6/Si(111)-(7×7) configuration (see Figure 3(e)). Here, 0.5V positive bias voltage are adopted in both cases. Schematic diagram on top of the figure illustrates the location of the unfaulted (U) and faulted (F) halves within the 7×7 unit cell. The using of the experimental STM image presented here is authorized by Elsevier.