

Electronic Supplementary Information

Isolated and Assembled Silver Aggregates on the Si(001) Surface: The Initial Stage of Film Formation

Kai Huang,^{1,*} Xiaohang Huang,¹ and Jun Nogami^{2,*}

¹ Chemistry Program, Guangdong Technion Israel Institute of Technology, 241 Daxue Road, Shantou, Guangdong Province, 515603, China

² Department of Materials Science and Engineering, University of Toronto, 184 College Street, Toronto, Ontario, M5S 3E4, Canada

* Corresponding authors: kai.huang@gtit.edu.cn and jun.nogami@utoronto.ca

S1 Additional DFT Results

In Figure S1, we present the ball-and-stick models of clean Si(001) and isolated Ag-aggregates in top view (left), front view (middle) and back view (right) so as to visualize the positions of underlying substrate atoms.

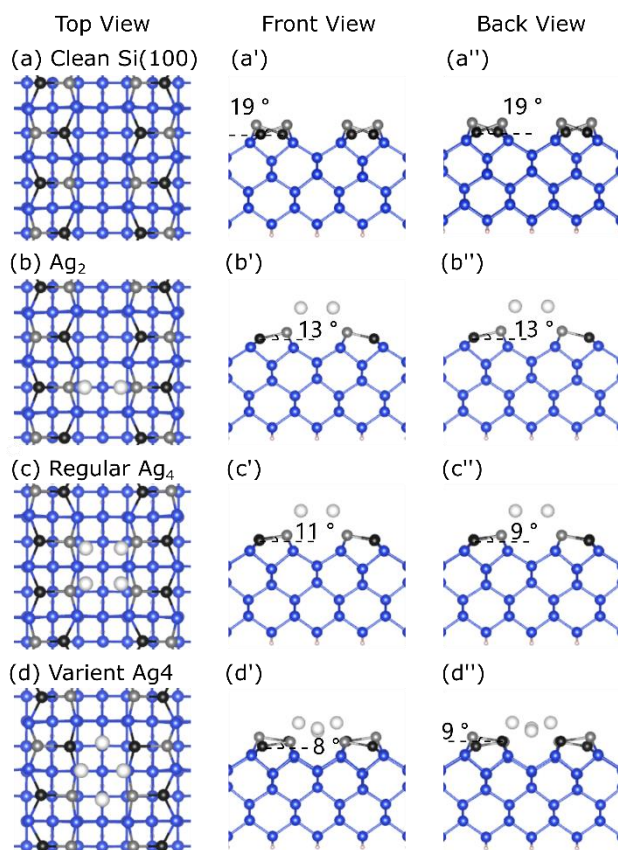


Figure S1 The ball-and-stick models of clean Si(001) and isolated Ag-aggregates in top view (left), front view (middle) and back view (right).

In Figure S2, we present the ball-and stick models of the Ag-chain and the Ag-film in top view (left) and side view (right) so as to visualize the positions of underlying substrate atoms.

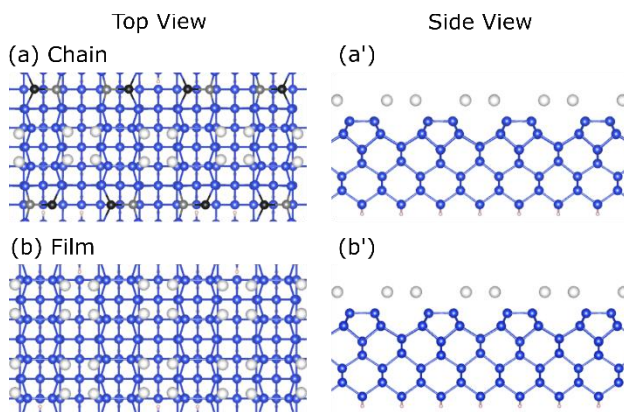


Figure S2 the ball-and stick models of the Ag-chain and the Ag-film in topview (left) and sideview (right)

The variant Ag-tetramer adopts two equivalent configurations, as in Figure S3a - b'. A reversible switch between these two configurations is of a computed barrier of ~ 0.18 eV, by the climbing image nudged elastic band technique.¹ Given the known overestimation of ~ 0.1 eV in the stabilization of buckled Si-dimers by DFT,² this would bring the value down to as small as ~ 80 meV. At 100-140 K, this switch process occurs rather fast, giving an “averaged” symmetric appearance as in Figure S3c’.

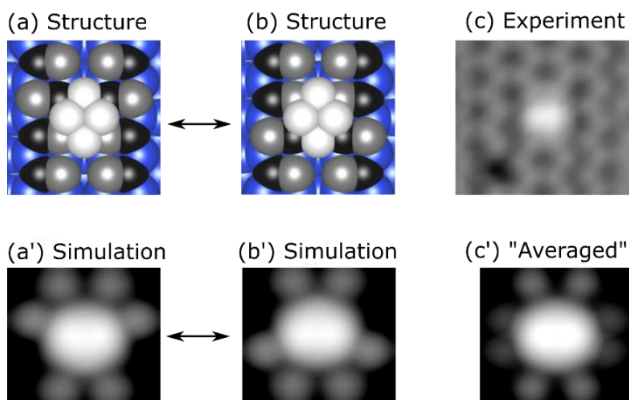


Figure S3 The reversible switching process of the variant tetramer between two equivalent configurations, (a) and (b). The corresponding simulated STM images are given in (a') and (b'). This process occurs rather fast at 100-140 K, giving a symmetric appearance as in (c) experiment and (c') simulated “averaged” STM image.

S2 Additional STM Results

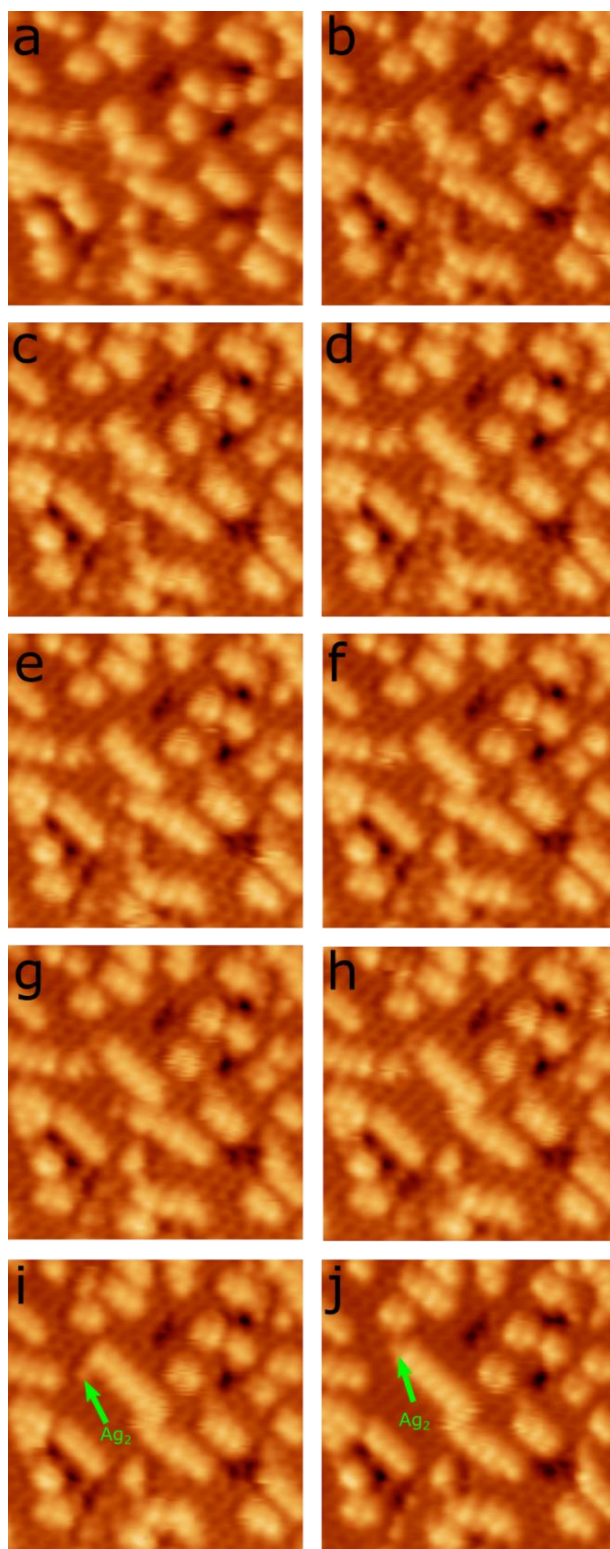


Figure S4 Evolution of Ag-aggregates into chains on Si(001) at 140 K. Panel (a) represents the first image of this region, which was recorded by time-lapsed STM at a delay of (b) 3:09 (hour: minute), (c) 6:53, (d) 8:33, (e) 17:31, (f) 19:42, (g) 23:12, (h) 27:44, (i) 30:02, and (j) 37:53. Panel (i) and (j) show the growth of a silver chain by the migration of a Ag-dimer. In all panels, imaging parameters are as follows: -2.5 V, 35 pA, 140 K, 132 x 132 Å².

Reference

¹ G. Henkelman and H. Jónsson, *J. Chem. Phys.*, 2000, **113**, 9901-9904.

² S. B. Healy, C. Filippi, P. Kratzer, E. Penev, and M. Scheffler, *Phys. Rev. Lett.*, 2001, **87**, 016105