Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information for

Density Functional Theory Study on Organically Surface-Modified Silicene

Rong Wang,[1,2] Xiaodong Pi,[1] Zhenyi Ni,[1] Yong Liu[1] and Deren Yang[1]*

[1]State Key Laboratory of Silicon Materials and Department of Materials Science and Engineering, Zhejiang University, Hangzhou 310027, China

[2] Key Laboratory of Interface Science and Engineering in Advanced Materials, Ministry of Education, Taiyuan University of Technology, Taiyuan 030024, China

Email: xdpi@zju.edu.cn

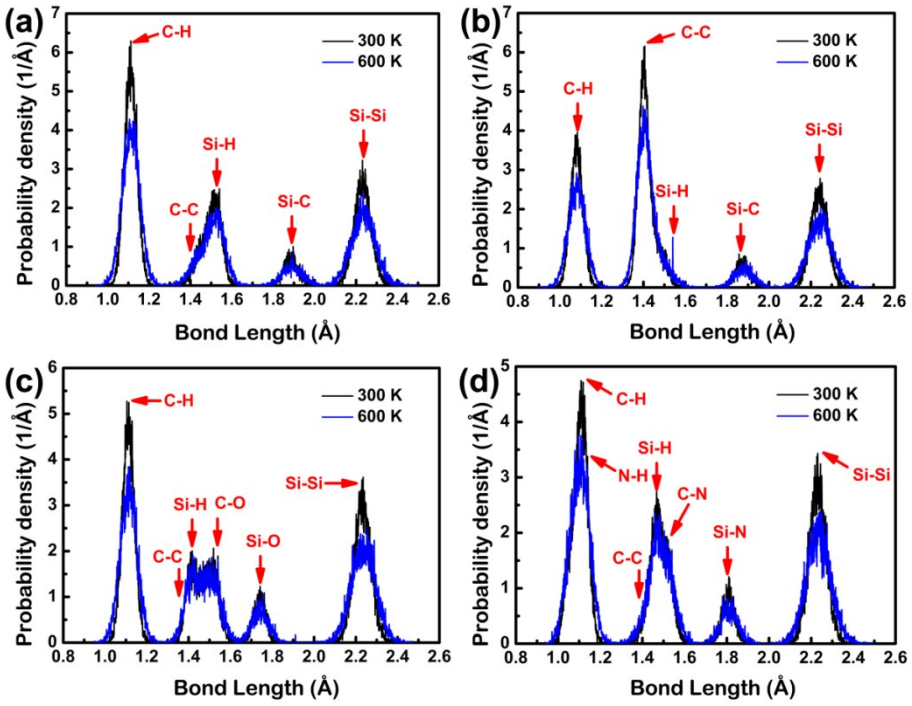

Fig. S1. Bond distributions of (a) hydrosilylated silicene, (b) phenylated silicene, (c) alkoxylated silicene and (d) aminated silicene at 300 and 600 K after 2000 ps of molecular dynamics.

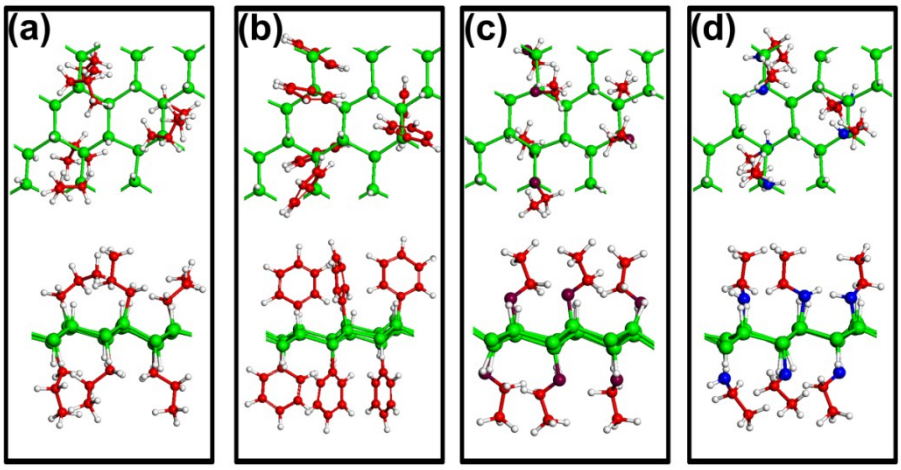

Fig. S2. Structures of (a) hydrosilylated silicene, (b) phenylated silicene, (c) alkoxylated silicene and (d) aminated silicene at 600 K after 2000 ps of molecular dynamics. Both top and side views of each structure are shown. Si, H, C, O and N atoms are denoted by green, white, red, purple and blue balls, respectively.

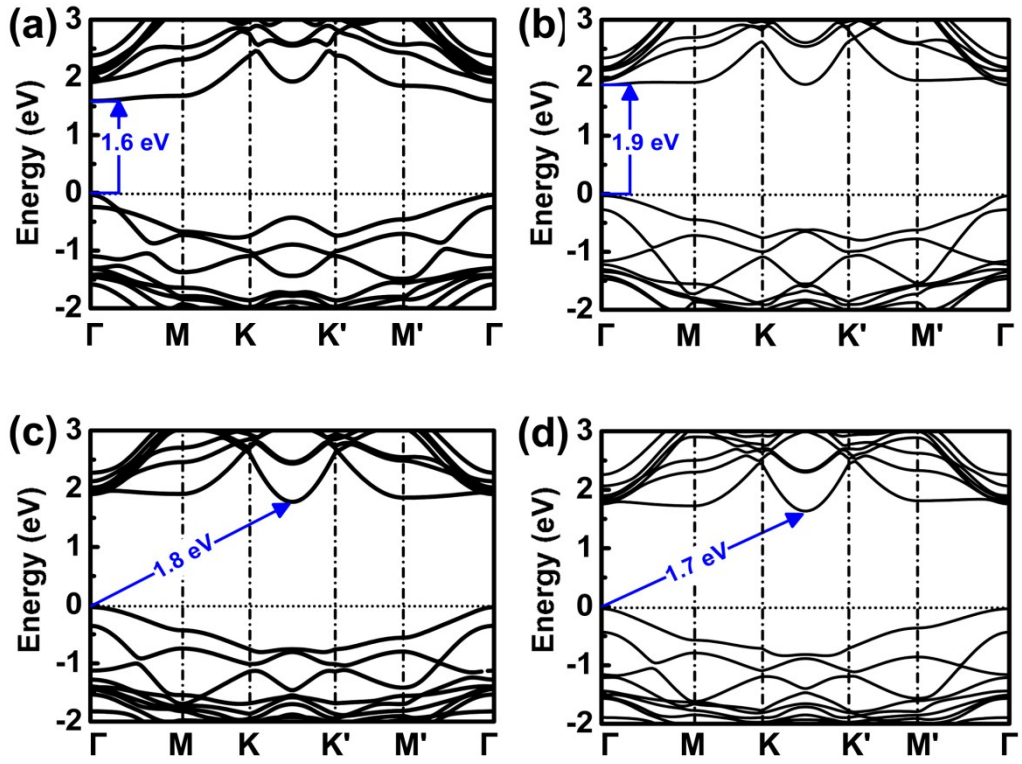

Fig. S3. Band structures of propylene-hydrosilylated silicene with the surface coverages of (a) 5%, (b) 11%, (c) 33% and (d) 44%. Energy is shifted so that the Fermi level is at 0 eV.