Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Microscopic origin of the π states in epitaxial silicene on $ZrB_2(0001)$[1] ANTOINE FLEURENCE, JAIST, YASUO YODHIDA, ISSP, University of Tokyo, CHI-CHENG LEE, TAISUKE OZAKI, JAIST, YUKIO HASEGAWA, ISSP, University of Tokyo, YUKIKO YAMADA-TAKAMURA, JAIST — Silicene, the graphene-like allotrope of silicon is the object of a recently raised enthusiasm, due to the perspectives opened by the novelty of its electronic, physical and chemical properties deriving from its π electronic system. So far, silicene only exists in epitaxial forms on metallic substrates. In particular, the spontaneous and self-terminating segregation of silicon atoms on the (0001) surface of zirconium diboride (ZrB_2) thin films epitaxied on Si(111) gives rise to a wide-scale uniform ($\sqrt{3} \times \sqrt{3}$)-reconstructed two-dimensional silicene sheet [1]. By means of low-temperature scanning tunneling spectroscopy and density functional theory calculations, we investigated the impact of the buckling of epitaxial silicene at atomic scale on the electronic properties. The microscopic origin of the valence and conduction states was determined and the strong contribution of the p_z orbitals of specific Si atoms to those states demonstrate their π character. A clear correlation between the estimated orbital hybridization of the Si atoms and the buckling was also found.
[1]: A. Fleurence et al., Phys. Rev. Lett., 108, 245501 (2012)

[1]This work was supported by KAKENHI (No. 24810011), NEXT program (GR046), and also by the joint research program of the Institute for Solid State Physics, the University of Tokyo.

Antoine Fleurence
JAIST

Date submitted: 15 Nov 2013 Electronic form version 1.4