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A planar-like silicene on $ZrB_2(0001)$ surface revealed by a first-principles study CHI-CHENG LEE, YUKIKO YAMADA-TAKAMURA, TAISUKE OZAKI, School of Materials Science, Japan Advanced Institute of Science and Technology (JAIST), 1-1 Asahidai, Nomi, Ishikawa 923-1292, Japan — Given that a free standing planar silicene is unstable [1], it is of great interest to understand the mechanism of stability of any existing planar-like structure that would optimize the understanding of the intrinsic difference from its counterpart, graphene. Recently, silicene was epitaxially grown on the $ZrB_2(0001)$ surface and was demonstrated to have $(\sqrt{3} \times \sqrt{3})$-reconstruction due to irregular buckling [2]. While the deviation from the regularly buckled structure is clearly made by experiment, two possible structures revealed by a first-principles calculation are still in the candidate list, neither one is completely ruled out from the possible groundstate structure. The energetically more favorable one possesses a planar-like structure, with all Si atoms residing in a plane except the one on top of a Zr atom becomes higher. However, this structure is less preferable from available experimental data. By studying the binding energy and electronic band structures of these two structures with and without the substrate, we will explain why such a planar-like structure can gain more energy than the regularly buckled-like phases via the interaction of the $ZrB_2(0001)$ surface and why the ground state advocated by density functional theory could become less preferable by experiment. [1] S. Cahangirov *et al.*, Phys. Rev. Lett. **102**, 236804 (2009). [2] A. Fleurence *et al.*, Phys. Rev. Lett. **108**, 245501 (2012).

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