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Novel two-dimensional silicon and germanium allotropes: a first-principles study FLORIAN GIMBERT, CHI-CHENG LEE, RAINER FRIEDLEIN, ANTOINE FLEURENCE, 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 — Graphene has been extensively studied but its integration into Si-based device technologies is difficult. It has been recently predicted by first-principles calculations that freestanding silicene and germanene, the counterparts of graphene made of Si and Ge atoms respectively, have graphene-like electronic structure with a low buckled structure [1]. So far, the models predicted by first-principles calculations were not able to describe completely the experimental results. These difficulties tend to suggest a more complex phase diagram for freestanding silicene or for silicene on a substrate than the simple buckled phase. We report for the first time a novel two-dimensional silicon and germanium allotropes, with a structure similar of that of MoS_2 layer [2]. After investigating a large range of lattice constants by first-principles calculations with OpenMX code, we show that this structure is the ground state for freestanding two-dimensional silicon and germanium layers instead of the usually considered low buckled silicene and germanene.

[1] S. Cahangirov et *al.*, Phys. Rev. Lett. **102**, 236804 (2007).
[2] B. Radisavljevic et *al.*, Nature Nano. **6**, 147 (2011).

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