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Bismuth-aluminum two-dimensional 2×2 compound and its ordered 9×9 domains on Si(111) surface

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### ACCEPTED MANUSCRIPT

## **Highlights**

- The only 2x2 structure can cover the entire surface in the (Bi,Al)/Si(111) system.
- The 2x2 can be formed in the wide range of temperature, from RT to 500°C, depending on the initial surface.
- The 2x2 can cover the surface with small-sized domains, ordered domains and large-sized domains, depending on the way of formation.
- A 500°C annealing orders the 2x2 domains to the 9x9 superstructure.
- Atomic model of the 2×2 has been discovered using *ab-initio* random structure searching method; the model has the only symmetry, mirror  $\sigma_v$  symmetry.

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