

## Fracture of two-dimensional structures of silicon – molecular dynamics simulation

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Due to their large flexibility and promising mechanical and electrical properties, two-dimensional(2D) nanomaterials such as graphene, GaSe and Bi<sub>2</sub>Se<sub>3</sub> have been vigorously studied over the past a few decades [1-2]. Especially, vast progress of graphene drove people to exploit other atoms in the IV group, (e.g. Si and Ge) in order to produce similar structure of 2D materials: silicene and germanene [1]. With hydrogen passivated, silicene and germanene turn to be silicane and germanane, respectively, which would be direct gap semiconductors [2] [3].

Though being promising electrical materials, it is also important to understand the mechanical properties of silicene and silicane for the reliable functioning and manufacturing. However, only a few research papers [4] [5] have been published on the mechanical properties of silicene and silicane to the best knowledge of the authors. In this study, using molecular dynamics simulations, we have performed tensile and bending test of silicene and silicane to study their deformation behavior and failure patterns.

The interactions between Si-Si, Si-H, and H-H are described by a bond order potential model of Murty and Atwater [6].

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