Abstract Submitted
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Radial Distribution Function of Silicene[1] MA. RAYO CHAVEZ-CASTILLO, Instituto de Fisica BUAP, MARIO ALBERTO RODRIGUEZ-MEZA, Depto. de Fisica, ININ, LILIA MEZA-MONTES, Instituto de Fisica BUAP — Silicene is the counterpart of graphene and its potential applications as a part of the current electronics, based in silicon, make it a very important system to study. We perform molecular dynamics simulations and analyze the structure of two and three dimensional arrays of Si atoms by means of the radial distribution function at diferent temperatures and densities. As a first approach, for the 2D case, the Lennard-Jones potential is used and two sets of parameters are tested. We found that the radial distribution function does not change with the parameters and resembles the corresponding to the (111) surface of the FCC structure, which is similar to that of the honeycomb lattice although with different peak heights. The liquid phase appears at very high temperatures, suggesting a very stable system in the solid phase. In 3D, a comparison with potentials developed specifically for silicon, as suggested by Stillinger and Weber[F. H. Stillinger and T. A. Weber, Phys. Rev. B 31, 5262 (1985)] will be presented.

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