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First-principles prediction of the structural, electronic and vibrational properties for t-silicene[1] EDUARDO CIFUENTES-QUINTAL, ROMEO DE COSS, Department of Applied Physics, Cinvestav-Merida, Mexico — With the synthesis of graphene and the discovery of its amazing properties, the research and the design for new 2D-materials began. In this line, silicene (silicon analogous to graphene) becomes very attractive because most of the current technology is already based on silicon. Therefore, the discovery of new silicon based 2D-materials with different properties could be helpful. In this work we have studied the vibrational stability for a new two-dimensional silicon allotrope based on buckled tetrarings (T-silicene). Our results were obtained within the framework of the density functional perturbation theory, using the plane-wave pseudopotential method, and the GGA-PBE96 exchange-correlation functional. We found that, in analogy to hexagonal Silicene, plane and buckled T-silicene are energetically stables. However, plane T-silicene shows imaginary phonon frequencies, and therefore is vibrationally unstable. Thus, buckled T-silicene is vibrationally stable and presents metallic character. More interestingly, the electronic structure shows that the energy bands crossing the Fermi level have a linear behavior with the wave vector. We will present a detailed analysis of this feature.

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