

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Young's Modulus of bilayer Silicene Nanoribbons¹ LILIA MEZA-MONTES, M. R. CHÁVEZ-CASTILLO, Instituto de FBUAP, Mexico, M. A. RODRÍGUEZ-MEZA, Instituto Nacional de Investigaciones Nucleares, Mexico — Mechanical properties of Silicene Nanoribbons (SNRs) are determined by their width and chirality, and can be also be modified by the presence of vacancy defects [1]. In the case of bilayer SNRs, interlayer interactions influence its physical properties [2]. We report results, at room temperature, on the Young's Modulus (YM) of pristine and monovacancy defective bilayers of SNRs. Molecular dynamics simulations were performed using the EDIP potential [3, 4]. YM increases with SNRs length, depends on chirality, the number and location of vacancies. Distance between layers is also important. These results are discussed in terms of missing bonds. Atomic stress distributions for defective bilayer SNRs show a larger stress concentration around the vacancy defect. Besides, if only the second layer has a mono-vacancy at its center, a larger stress concentration is observed on the atom located just below the vacancy defect. Thus, the bilayer structure carries less strain and it can be easily deformed.

[1] M. R. Chávez-Castillo *et al.*, RSC Adv., 5, 96052 (2015).

[2] T. Morishita *etal.*, Chem. Phys. Lett. 506, 221 (2011).

[3] Steve Plimpton, Comput. Phys. 117, 1 (1995).

[4] João F. Justo, et al., Phys. Rev. B 58, 5, 2539 (1998).

¹Partially supported by VIEP-BUAP, Mexico.

Lilia Meza-Montes
Instituto de Fisica BUAP, Mexico

Date submitted: 11 Nov 2016

Electronic form version 1.4