

Accepted Manuscript

First-principles investigation on defect-induced silicene nanoribbons
– A superior media for sensing NH₃, NO₂ and NO gas molecules

Gurleen Kaur Walia , Deep Kamal Kaur Randhawa

PII: S0039-6028(17)30697-0
DOI: [10.1016/j.susc.2017.12.013](https://doi.org/10.1016/j.susc.2017.12.013)
Reference: SUSC 21169



To appear in: *Surface Science*

Received date: 19 September 2017
Revised date: 17 December 2017
Accepted date: 23 December 2017

Please cite this article as: Gurleen Kaur Walia , Deep Kamal Kaur Randhawa , First-principles investigation on defect-induced silicene nanoribbons – A superior media for sensing NH₃, NO₂ and NO gas molecules, *Surface Science* (2017), doi: [10.1016/j.susc.2017.12.013](https://doi.org/10.1016/j.susc.2017.12.013)

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Highlights

- The band gap of pristine armchair silicene nanoribbons (ASiNR) is tuned by introducing defect.
- Defective ASiNR is suitable as an ideal sensor for NH_3 , NO_2 and NO gas molecules.
- NH_3 , NO_2 and NO behave as electron-donating gases, donating electronic charge to ASiNR.
- Electronic and transport properties of ASiNR-molecule complexes are studied.

ACCEPTED MANUSCRIPT

Download English Version:

<https://daneshyari.com/en/article/7844802>

Download Persian Version:

<https://daneshyari.com/article/7844802>

[Daneshyari.com](https://daneshyari.com)