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Author: Junhui Yuan Qingxing Xie Niannian Yu Jiafu Wang

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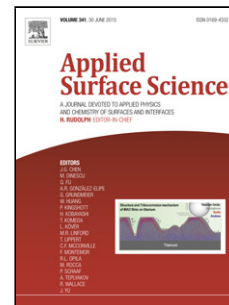
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# Surface Regulated Arsenenes as Dirac Materials: From Density Functional Calculations

Junhui Yuan Qingxing Xie Niannian Yu\* Jiafu Wang\*

School of Science, Wuhan University of Technology, Wuhan, Hubei, 430070, China

\*Corresponding Authors.

Email Addresses: [niannianyu@whut.edu.cn](mailto:niannianyu@whut.edu.cn) (N.Yu), [jasper@whut.edu.cn](mailto:jasper@whut.edu.cn) (J. Wang)

## Highlights:

- By first-principles calculations, we have revealed the presence of Dirac cones in chemically decorated buckled arsenene AsX (X = CN, NC, NCO, NCS, and NCSe), and all these chemically decorated arsenenes could spontaneously form and would be stable in defying thermal fluctuations in room temperature.

## Abstract

Using first principle calculations based on density functional theory (DFT), we have systematically investigated the structure stability and electronic properties of chemically decorated arsenenes, AsX (X = CN, NC, NCO, NCS and NCSe). Phonon dispersion and formation energy analysis reveal that all the five chemically decorated buckled arsenenes are energetically favorable and could be synthesized. Our study shows that wide-bandgap arsenene would turn into Dirac materials when

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