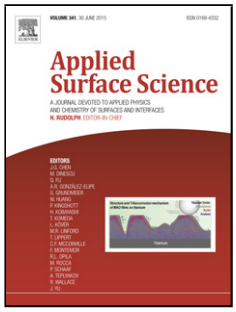

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Surface Regulated Arsenenes as Dirac Materials：From Density Functional Calculations

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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 defending 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