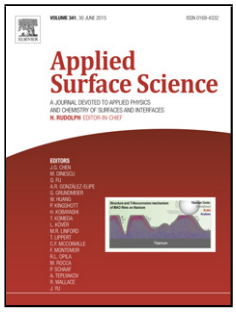

Title: Electric field <!–<query id="Q1">Please check the ḊOC headf̈or correctness.</query>–>improved the sensitivity of CO on substitutionally doped antimonene

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Electric field improved the sensitivity of CO on substitutionally doped antimonene

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Highlights.

- The properties of doped antimonene have been studied by DFT calculations.
- All doping processes are exothermic and thermodynamically possible.
- Doped antimonene has an enhanced chemical activity for the CO molecule.
- An external electric field could improve the CO gas sensitivity of the antimonene.

Abstract

The geometrics and electronic structures of substitutionally doped antimonene and the interaction between CO molecule different substrates have been investigated using first-principles calculations to exploit the sensitivity of CO to antimonene. It is found that CO adsorption on pristine antimonene is physical adsorption, while it is converted to chemical adsorption after doping. The results indicate that an external electric field (*V*) ranges from -0.5 eV/Å to 0.21 eV/Å could improve the CO gas sensitivity of the antimonene, which is helpful to realize the use of CO gas sensor at room temperature.

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