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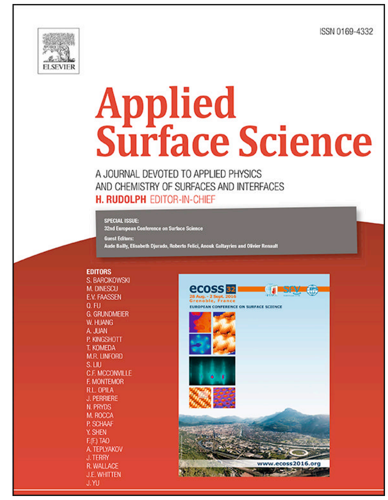

Full Length Article

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PII: S0169-4332(18)32395-X
DOI: https://doi.org/10.1016/j.apsusc.2018.08.252
Reference: APSUSC 40289

To appear in: *Applied Surface Science*

Received Date: 27 June 2018
Revised Date: 22 August 2018
Accepted Date: 28 August 2018

Please cite this article as: S. Dai, Y-L. Lu, P. Wu, Tuning electronic, magnetic and optical properties of Cr-doped antimonene via biaxial strain engineering, *Applied Surface Science* (2018), doi: https://doi.org/10.1016/j.apsusc.2018.08.252

Tuning electronic, magnetic and optical properties of Cr-doped antimonene via biaxial strain engineering

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Abstract

Our work develops a novel pathway for controllable and tunable spintronics and optoelectronics devices. The biaxial strain and doing functions on electronic structure, magnetic and optical properties were explored with the method of density functional theory (DFT). Results show that the Cr-doped antimonene is a narrow indirect band-gap semiconductor (0.44 eV), and the valence band maximum (VBM) changes from K to Γ point due to spin-orbit coupling (SOC) interaction. Hence, there exists a remarkable spin splitting near E_F caused by the coexistence of strong *p*-*d* hybridization and SOC effect. The total net magnetic moment is 3.00 μ_B in Cr-doped antimonene system, while the coupling interaction between them is anti-ferromagnetism (AFM) order, which facilitates its use in AFM-based spintronic devices. For the case of coexistence of strain and Cr dopant, the Cr-doped system transforms from magnetic semiconductor to magnetic half-metal material under the biaxial tensile strain of 6%. Most interestingly, the band gap closing can be achieved when biaxial strains range from -4% to -6%, so these systems present metal characteristics. Comparing with the unstrained doping system, the local magnetic

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