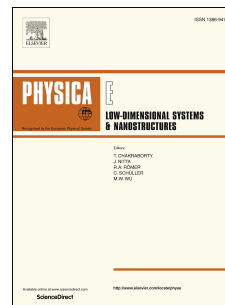


# Accepted Manuscript

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Jiansheng Dong, Yipeng Zhao, Gang Ouyang



PII: S1386-9477(18)30930-5

DOI: [10.1016/j.physe.2018.08.025](https://doi.org/10.1016/j.physe.2018.08.025)

Reference: PHYSE 13270

To appear in: *Physica E: Low-dimensional Systems and Nanostructures*

Received Date: 24 June 2018

Revised Date: 13 August 2018

Accepted Date: 21 August 2018

Please cite this article as: J. Dong, Y. Zhao, G. Ouyang, The effect of alloying on the band engineering of two-dimensional transition metal dichalcogenides, *Physica E: Low-dimensional Systems and Nanostructures* (2018), doi: 10.1016/j.physe.2018.08.025.

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**The effect of alloying on the band engineering of two-dimensional transition  
metal dichalcogenides**

Jiansheng Dong, Yipeng Zhao, and Gang Ouyang\*

*Key Laboratory of Low-Dimensional Quantum Structures and Quantum Control of  
Ministry of Education, Synergetic Innovation Center for Quantum Effects and  
Applications (SICQEA), Hunan Normal University, Changsha 410081, China*

**Abstract**

In order to clarify the alloying effect on the band engineering in two-dimensional transition metal dichalcogenides (2D-TMDs) at the atomic level, we present a quantitative study to address a deeper insight on the relationship between the bond identities and band shift based on the bond relaxation mechanism and valance-force-field approach. We find the interaction parameter in 2D-TMDs alloys could be obtained from the lattice distortion energy and further reveal the bowing mechanism of composition tunable bandgap in 2D-TMDs. Our results show that the composition-dependent band shift is in good agreement with the available evidence, which suggest the tunable electronic properties of 2D-TMD alloys that realized by modulating the chemical composition could be helpful for nanoelectronic applications.

\* Corresponding author: [gangouy@hunnu.edu.cn](mailto:gangouy@hunnu.edu.cn)

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