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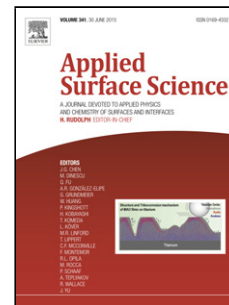
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Authors: M. Meng, C.G. Shi, T. Li, S.E. Shi, T.H. Li, L.Z. Liu

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Magnetism induced by cationic defect in monolayer ReSe₂ controlled by strain engineering

M. Meng¹, C. G. Shi⁴, T. Li², S. E. Shi^{1,2}, T. H. Li^{2,a)}, and L. Z. Liu^{3,a)}

¹*College of Physics and Telecommunication Engineering, Zhoukou Normal University, Zhoukou, Henan, 466001, China*

²*College of Electronic Engineering, Guangxi Normal University, Guilin 541004, People's Republic of China*

³*Microstructures, National Laboratory of Solid State Microstructures, Nanjing University, Nanjing 210093, P. R. China*

⁴*College of Chemistry and Chemical Engineering, Nantong University, Nantong, 226019, P. R. China*

Highlights

- Symmetry breaking is achieved by defect introduction that modulates its electronic structure.
- Redistribution of electronic cloud induced by cationic defect leads to desirable magnetism.
- Combined action of defect and strain causing its magnetism modification

Abstract

The formation and regulation of magnetism has attracted much attention because of its potential application in spintronics. The magnetic properties and electronic structure of ReSe₂ with cationic defect under external strain are determined theoretically based on the density function theory. The tensile deformation induced by external strain not only leads to changes in defect formation energy but also regulate the magnetic characteristics. However, as compressed deformation induced by external strain increases, the magnetism in the structure with cationic defect will disappear sharply. It is interesting to note that the anionic defect cannot give rise to

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