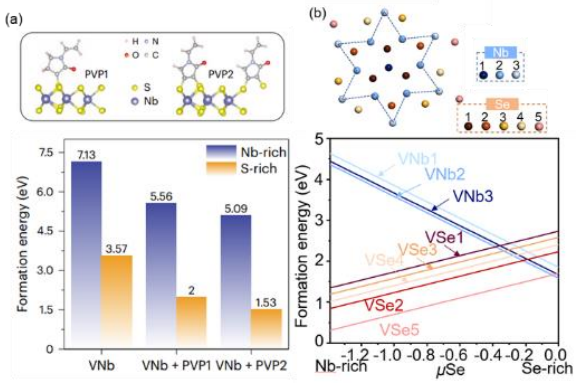
Defect engineering in monolayer transition metal dichalcogenides

Mengmeng Niu [1,*] Jingsi Qiao [1],Yeliang Wang[1]
[1] Beijing Institute of Technology, Beijing, China
*email: mengmniu@bit.edu.cn

Abstract

Atomically precise defect engineering is an effective method to modulate the physical properties of transition metal dichalcogenides (TMD), making them promising candidates for various applications, including electronics, optoelectronics, and catalysis, etc. However, constructed precise vacancies, especially metal vacancies, are limited. The effect of defects on electron-correlated properties is poorly understood. Recently, precisely fabricating metal and chalcogen vacancies in TMD has been achieved by molecular modification.[1] Besides, we investigated the properties of 1T-$NbSe_2$ charge density wave (CDW) monolayer with various single Se/Nb vacancy using density functional theory calculations.[2] We found a unique Se vacancy site, called magic Se vacancy, could precisely erase the Mott electrons. Besides, Mott electrons could be more flexibly manipulated when the magic Se site is substituted with As, Br and K elements. The electronic properties of 1T-$NbSe_2$ with defects are tuned by the synergistic effect of compressive strain and electron doping. Our findings reveal that defect engineering is an ingenious strategy for atomically manipulating electron-correlated properties and manufacturing electronic patterns, guiding to erase and write in Mott electrons in two-dimensional materials.



Pic.1. (a) Atomic models and formation energies of metal vacancy in pristine and PVP-capped 1H-NbS_2. (b) Eight types of vacancies in the Charge-Transfer insulator 1T-$NbSe_2$ supercell were considered.

Bibliography

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[2] **Niu M**, Dai J, Qiao J. et al. To be submitted (2024).