

Tuning the charge density waves and band structure in VSe₂ by Na intercalation

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Recent developments of 2D materials studies tend to understand the properties change between monolayers or few-layers compounds and their bulk counterpart. Transition Metal Dichalcogenides (TMD) are layered materials, among 2D materials, offering a vast field of investigation of properties resulting from such transition. Here, we focus on bulk 1T-VSe₂ which exhibits a 4x4x3 Charge Density Wave (CDW) below 120K and is predicted to be ferromagnetic at the monolayer scale [1]. We discuss first its band structure and the local electronic properties measured by Scanning Tunnelling Microscopy (STM). We observe a modification of the CDW when Na is intercalated, corresponding to the one identified for a monolayer [2]. At the junction between intercalated and non-intercalated VSe₂, a 1D 0 energy edge state arises. DFT calculations have been then carried to understand this specific interface and the subtle effect of doping.

References

- [1] Bonilla, M.; Kolekar, S.; Ma, Y.; Diaz, H.C.; Kalappattil, V.; Das, R.; Eggers, T.; Gutierrez, H. R.; Phan, M. H.; Batzill, M.; *Nature Nano*, Vol. 13, No. 4, 2018-04
- [2] Ekvall, I.; Brauer, H. E.; Wahlström, E.; Olin, H. *Physical Review B* 1999, 59, 7751-7761

Figures

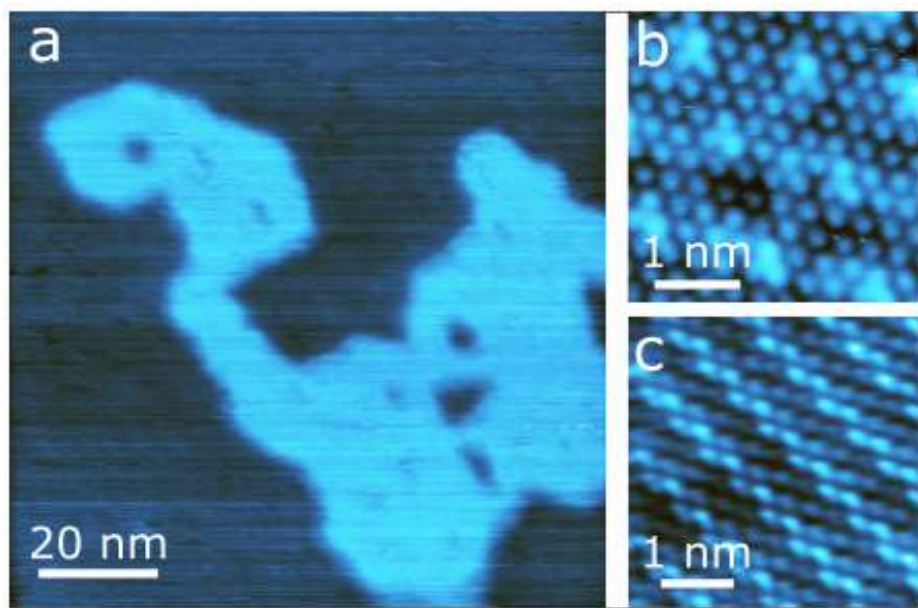


Figure 1: STM constant current image of Na intercalated VSe₂ surface (a), showing $\sqrt{3} \times \sqrt{7}$ CDW order (c), differing from the bulk 4 X 4 (b).