Electronic ground state evolution of single-layer $NbSe_2$ throughout the metal-semiconductor transition by substitutional doping.

Rishav Harsh
Wen Wan, Paul Dreher and Miguel M. Ugeda
Donostia International Physics Center, Paseo Manuel de Lardizabal, 4, Donostia-San Sebastian, Spain
rishav.harsh@gmail.com

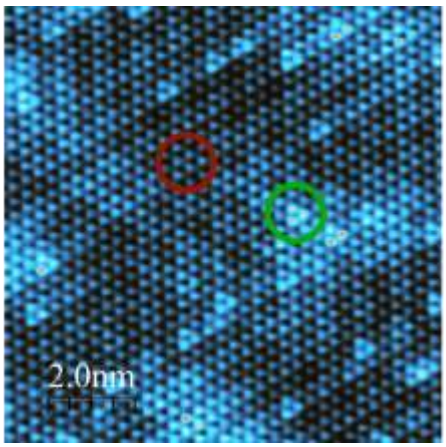
Substitutional doping is a robust method for modifying electronic and phononic properties of a crystal. Transition metal dichalcogenide (TMD) alloys offer unprecedented versatility to engineer 2D materials with tailored properties for specific purposes. The chalcogen and/or the transition metal atom can be substituted as an effective strategy. While substantial works have been reported on dilute 2D semiconducting alloys, 2D collective phenomena and correlated behavior in these TMD alloys remains largely unexplored. $NbSe_2$ is an ideal playground for the observation of collective electron phases such as superconductivity and charge density wave (CDW) order [1]. In this work [2], we report on the atomic-scale evolution of the electronic ground state of a monolayer of $Nb_{1-\delta}Mo_{\delta}Se_2$ with $0<\delta<1$ by means of low-temperature (300 mK) scanning tunneling microscopy/spectroscopy (STM/STS). In particular, we investigate the atomic and low-energy electronic structure of this 2D alloy throughout the metal to semiconductor transition from the monolayer of $NbSe_2$ to the monolayer of $MoSe_2$. Our STS measurements enable to extract the effective doping of Mo impurities, the bandgap evolution as well as the band shifts. Furthermore, we probe the existence and properties of collective electronic phases (CDW and superconductivity) to demonstrate remarkable robustness against impurities as well. Our results paint a clear and detailed picture of the evolution of the electronic structure in 2D TMD alloys.

References

[1] Ugeda, M., Bradley, A., Zhang, Y. *et al.*, Nature Phys., **12,** (2016) 92–97
[2] Wan, W., Dreher, P., Harsh, R. *et al.*, In preparation (2021).

Figures

1



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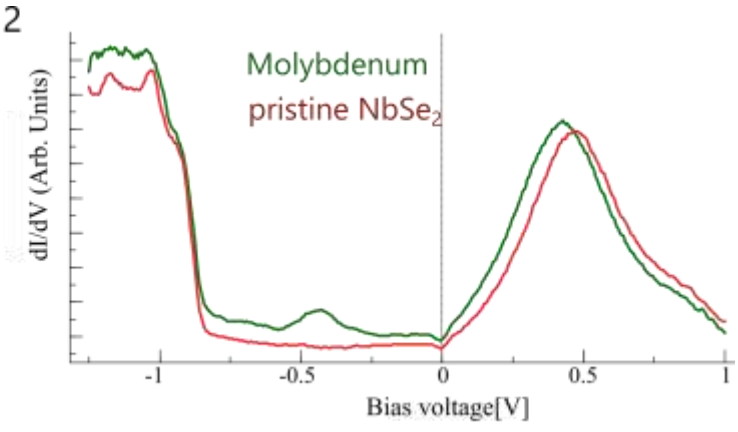

Figure (1) STM topography showing Mo defects in $NbSe_2$ lattice at doping level of 0.7% **(2)** STS comparison of pristine $NbSe_2$ lattice with the single atom Mo defect for the area shown in left.