

Coexistence of charge density wave phases in NbSe₂

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Abstract

NbSe₂ single-layers present a 3x3 charge density wave (CDW) order below 33 K^[1]. Due to its puzzling nature, the CDW state in this material has been at the core of a great deal of attention in recent years [2, 3]. In this study we combine density functional theory (DFT) calculations with low temperature scanning tunnelling microscopy (STM) to provide evidence for the existence of multiple CDW phases in its ground state. Our DFT studies show an abundant CDW state with the possible existence of up to 6 phases within a very narrow energy range. Low temperature STM (T = 1 K) measurements demonstrate the coexistence of two of the structural phases. Finally we show a remarkable agreement between the experimental STM images and DFT simulated ones.

References

- [1] M. M. Ugeda et al. Nature Physics 2016, 12, 92
- [2] C.-S. Lian et al. Nano Lett. 2018, 18, 2924
- [3] F. Zheng et al. PRB 2018, 97, 081101 (R)

Figures

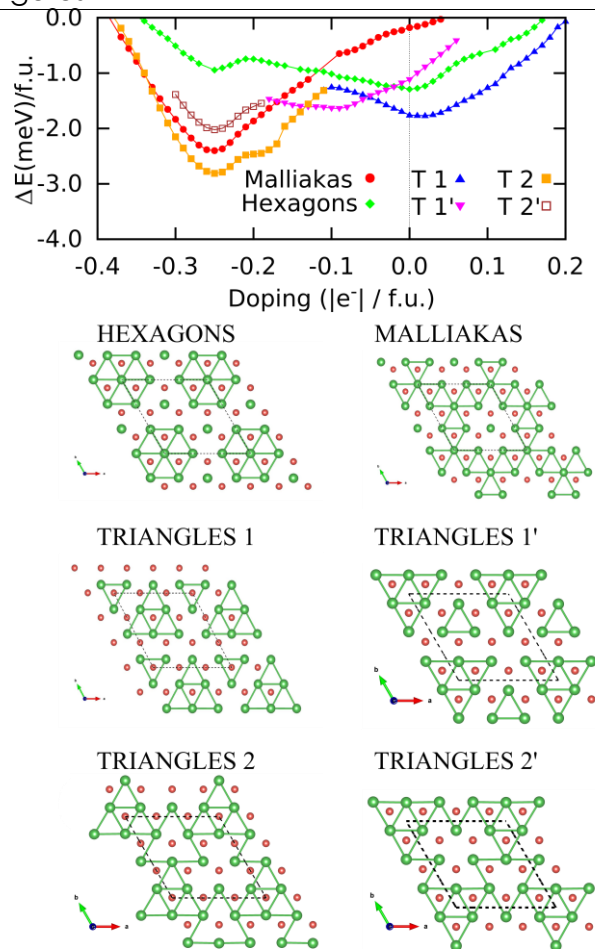


Figure 1: Different 3x3 CDW phases stability for a range of charge carrier doping levels. Energy differences are relative to the undistorted unit cell at their respective doping level. Green lines represent Nb-Nb bonds shorter than the ones in the undistorted structure.