二硒化鈮中的量子相：電荷密度波
Quantum Phase in Niobium Diselenide: Charge Density Wave

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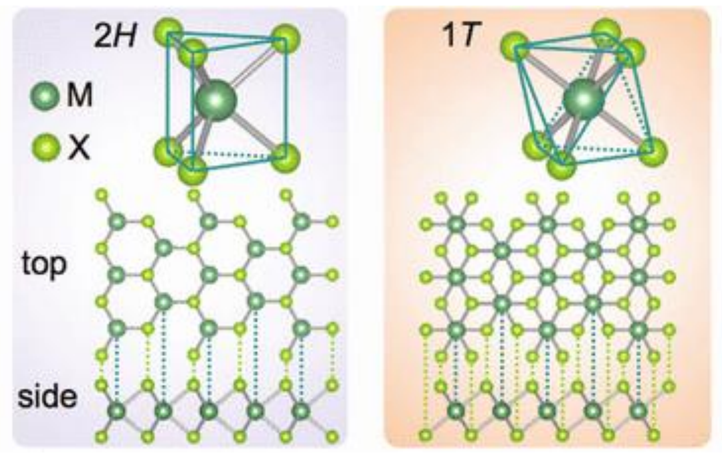
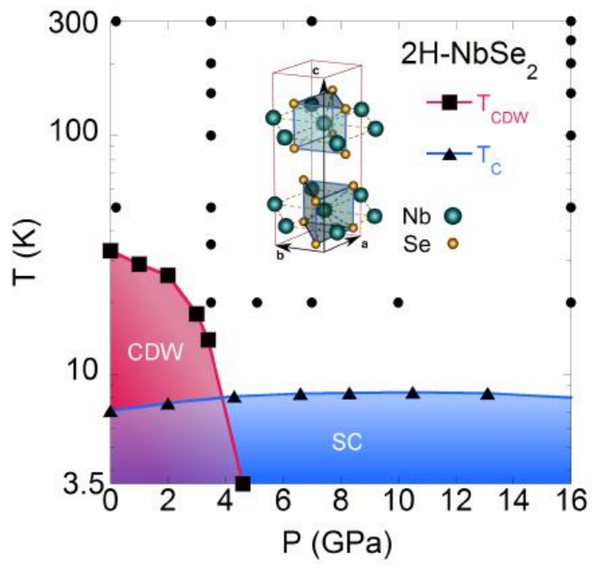
Introduction

As electronic devices getting smaller in scale, two dimensional materials were considered to have great potentialities, especially transition metal dichalcogenides (TMDs), a compound material made by the basis of one transition metal and two chalcogen atoms. TMDs are highly attractive since they are easier to fabricate based on their layered nature, and have a huge variety of possible combination creating wide material candidates for different application. When the materials were reduced in dimension, some intriguing phenomenon occurs, such as quantum phase transition in strong correlation system where electron-electron or electron-phonon interactions being the dominant internal mechanism, leads to superconducting phase and our main topic charge density wave (CDW). In the case of $NbSe_2$, just as other TMDs materials, has 2H and 1T two different structures, in low temperature under 10K, 2H-$NbSe_2$ displays a coexisting superconducting and (3×3)CDW phase, while $(\sqrt{13} \times \sqrt{13})$CDW was observed in 1T phase even at a high temperature above 200K, these fascinating properties have attracted dense studies and discussions.

In this work, we use scanning tunneling microscope (STM) to image the 1T-$NbSe_2$ surface and calculate the electronic structure throughout *ab initio* method, performed with Vienna Ab initio Simulation Package (VASP). We observed CDW at 77K, ultra-high vacuum (UHV), so we assume that 1T-$NbSe_2$ was observed. Band structure of primitive 1T-$NbSe_2$ were calculated.



Top view and side view of monolayer 2H-, 1T-$NbSe_2$ [1]



Superconducting-CDW-normal phase diagram of 2H-$NbSe_2$ [2]

Purposes

1. Surface topography of 1T-$NbSe_2$ observed by STM.
2. Band structure of 1T-$NbSe_2$ calculated by the *ab-initio* calculation.

Procedure and Method

1. STM measurement

STM imaging was performed using W tips at a liquid N_2 temperature (77 K). All images are analyzed by Gwyddion.

2. Ab-initio calculation

First-principles calculations were performed using the Vienna Ab Initio Simulation Package. The projector-augmented wave method and generalized gradient approximation were used to describe the exchange-correlation functional. The cut-off energy was set to 400 eV. A $18 \times 18 \times 1$ was adopted for 1×1 primitive cell, and a $4 \times 4 \times 1$ k-point mesh was used for R13 × R13 reconstruction supercell. To minic a $NbSe_2$ monolayer, a vacuum layer of 15 Å was applied.

Results and Discussion

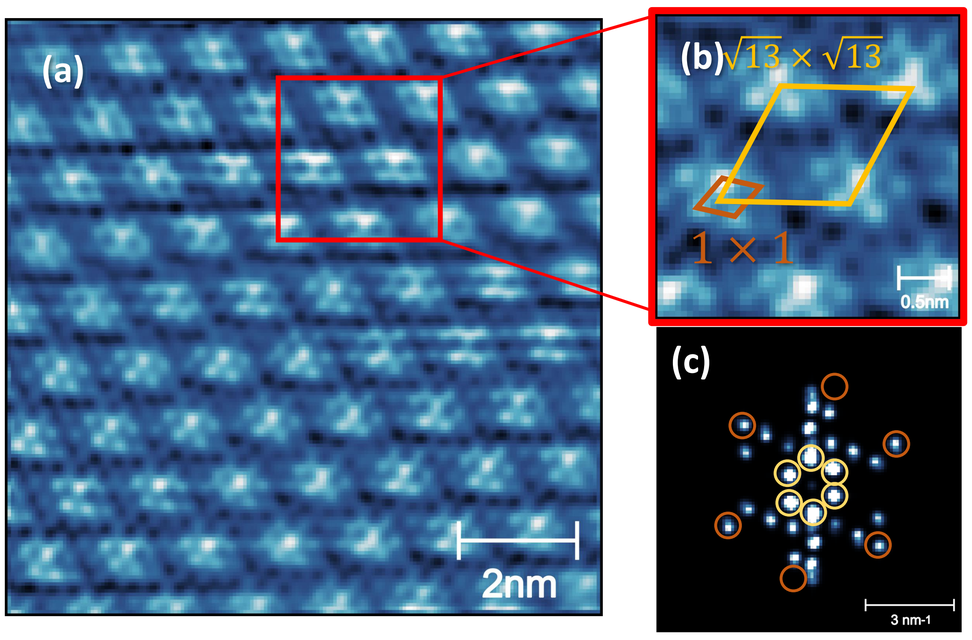


Fig. 1: (a) STM topography image of 1T-$NbSe_2$ surface (b) zoomed-in image of (a), orange unit cell indicates the 1×1 $NbSe_2$ periodicity, and the yellow one indicates the $\sqrt{13} \times \sqrt{13}$ CDW periodicity (c) Fast Fourier Transform (FFT) of STM image in (a), the orange and yellow circle point out the 1×1 $NbSe_2$ unit cell and $\sqrt{13} \times \sqrt{13}$ CDW , respectively

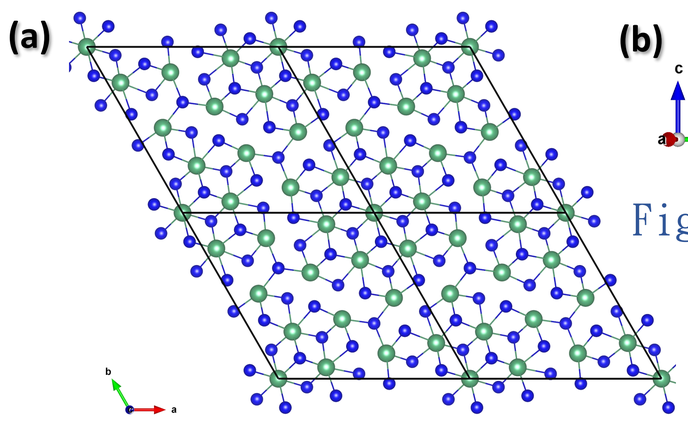


Fig. 2: (a) Top view and (b) side view of 1T-NbSe2 supercell for *ab-initio* calculation. The atomic model is based on [3].

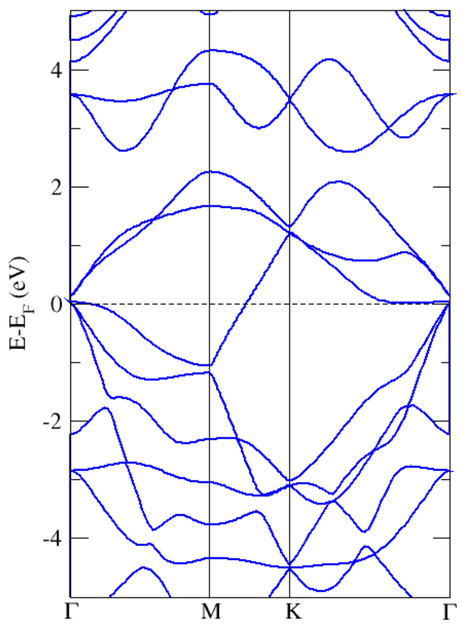


Fig. 3: Band structure of primitive cell, plotted along Γ－M－K－Γ high symmetry point

Reference

[1] Y. Nakata *et al.*, *NPG Asia Mater* **8,** e321 (2016).
[2] M. Leroux *et al.*, *Phys. Rev. B* **92**, 140303(R) (2015)
[3] M. Calandra, *Phys. Rev. Lett.* **121**, 026401 (2018)
[4] E. Kamil et al., *J. Phys.: Condens.* Matter **30** 325601 (2018)