



**S N BOSE NATIONAL CENTRE
FOR BASIC SCIENCES**

Block JD, Sector III, Salt Lake, Kolkata 700 106

DEPARTMENTAL SEMINAR

Condensed Matter and Materials Physics

12th February, 2024

4.00 PM

ONLINE/ FERMION

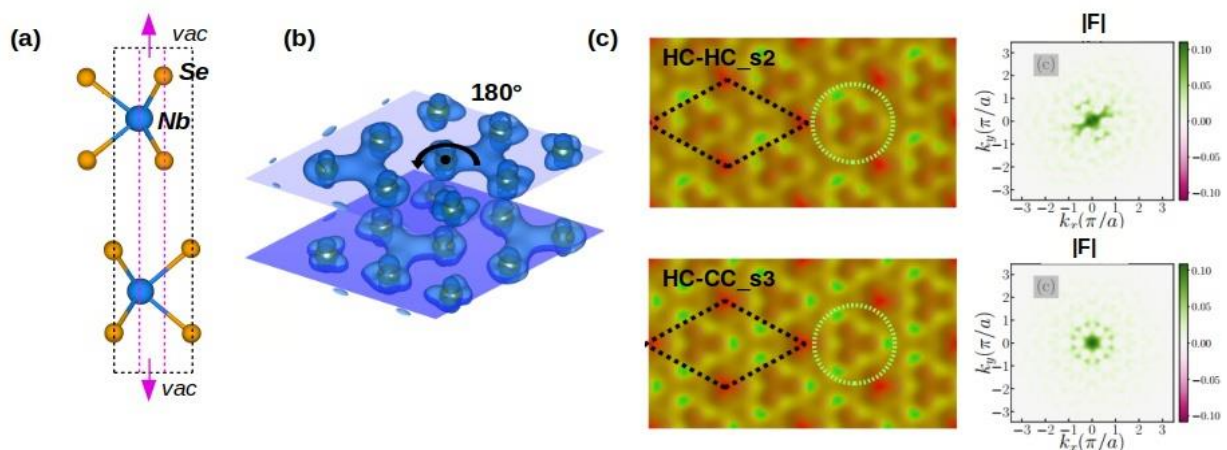
SPEAKER

Dr. Dhani Nafday
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Stockholm, Sweden

TITLE OF THE TALK

STACKING OF CHARGE DENSITY WAVES IN NBSE₂ BILAYERS

We employ ab-initio electronic structure calculations to investigate the charge-density waves and periodic lattice distortions in bilayer 2H-NbSe₂. We demonstrate that the vertical stacking can give rise to a variety of patterns that may lower the symmetry of the CDW exhibited separately by the two composing 1H-NbSe₂ monolayers. The general tendency to a spontaneous symmetry breaking observed in the ground state and the first excited states is shown to originate from a non-negligible inter-layer coupling. Simulated experimental patterns for scanning tunnelling microscopy (STM) and diffraction scattering show signatures of these different stacking orders which we speculate may be utilized to devise ad-hoc experiments for the investigation of the stacking order in 2H-NbSe₂. Finally, our results illustrate clearly that the vertical stacking is not only important for 1T structures, as exemplified by the metal-to-insulator transition observed in 1T-TaS₂, but seem to indicate that it is a general feature of metallic layered transition metal dichalcogenides as well.





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(a) Side view of the bilayer unit-cell stacking of BAB-CAC of the 2H type. (b) Example of a CDW charge distribution across two composing monolayers in the 2H NbSe₂ bilayer. (c) Simulated STM (left) and diffraction patterns (right). The images for the ground state CDW stacking distribution and the second excited state CDW stacking distribution are shown in the top row and bottom row respectively.

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HOST FACULTY

Dr. Arijit Haldar, Assistant Professor – Adjunct Faculty
