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Theoretical study of charge density wave in 1T-VSe2 heterostructures

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Charge density waves (CDWs) occur in many solids, in particular, in layered materials like transition metal dichalcogenides (TMDs). In bulk 1T-VSe2 the charge density modulation is known to be 4x4x3 with a 4x4 in-plane periodicity and three times the lattice vector out of the plane. However, for the monolayer or Na-intercalated VSe2 the CDW periodicity in the plane becomes √3R30x√7R19 [1]. Here, by means of density functional theory (DFT) calculations, with the Quantum ESPRESSO package, we systematically studied different CDWs in these systems. Calculated phonon dispersions were found to show imaginary frequencies at wave vectors corresponding to both 4x4 and √3R30x√7R19.1 superstructures pointing to associated instabiliy [2]. The related phonon displacement eigenvectors allowed us to set up supercell total energy calculations and obtain energy gains for comparison between different orderings. Next, combining ab initio localized orbitals code Fireball and the Keldysh-Green transport formalism, we have performed scanning tunneling microscopy (STM) simulations of different CDWs which were found to compare pretty well with experimental STM images. Finally, we have also investigated a 1T-VSe2 bilayer. We have found, in particular, that the √3R30x√7R19.1 CDW is more stable in the monolayer while the 4x4 one is more preferable energetically for the bilayer system, as observed experimentally [3].

References:
[1] Chazarin et al, Adv. Mater. Interfaces 2023, 10, 2201680
[2] Si et al, Physical Review B 2020, 101, 235405
[3] Chua et al, ACS Nano 2022, 16, 783-791

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