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Superlattices from defect engineering in two-dimensional semiconductors

Due to their unique electrical and optical properties, excitons in two dimensional materials are promising platforms for applications in optoelectronics, quantum information and quantum sensing. Excitons are bound states of electrons and holes in semiconductors and their control is crucial in many applications. Superlattices, artificial periodic structures with periods much larger than the unit cell dimension, can tune fundamental exciton properties, such as lifetime and interaction [1]. Localized excitons have been recently observed in moiré superlattices in heterostructures in which the geometry of the periodic potential is limited by the crystal lattice [2]. We propose to use defect engineering to modulate the band structure and thus tuning exciton energy profile by introducing structural defects in transition metal dichalcogenites (TMDs). Figure 1a shows the band structure of a pristine WS_2 supercell simulated using first principles density functional theory (DFT) [3], with quantum espresso package. When a 2% density of defect V_S (S vacancy) is introduced in the supercell (see Figure 1b), gap states (red color) reduce exciton energy of 0.31 eV creating a confining potential for excitons in the defective region. The choice of the types of defects and their concentration results in different potentials [4] and allowing designing arbitrary geometries and superlattice configurations. Recent advances in defect engineering in 2D materials, including atomic manipulation with electron microscopy [5], make now possible to create such defective superlattices. A possible squared configuration is presented in Figure 1c. This approach gives more freedom in modulating optical and electrical properties of the 2D materials and opens new pathways to control exciton dynamics for optoelectronic applications.

References

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Figures

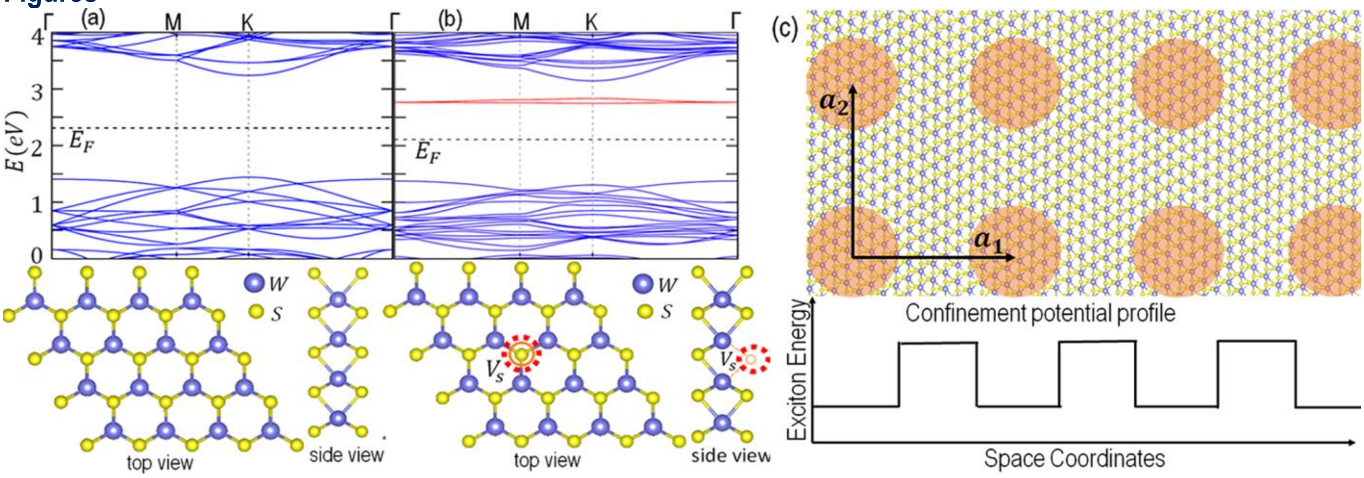

Figure 1: (a) band structure of pristine monolayer of WS2 with 4x4x1 supercell (b) band structure of monolayer of WS2 with 4x4x1 supercell with Vs vacancy (c) a possible example of superlattice and confining potential profile