

TMD nanoribbons: quasi 1D semiconductors with metallic edges

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Two-dimensional (2D) materials are promising candidates for sensing and optoelectronic applications. After the exfoliation of graphene and the discovery of its exceptional properties, several other 2D crystals have emerged. Prominent members of this group are single-layer transition metal dichalcogenides (TMDs) which among others include MoS₂, MoSe₂, WS₂ and WSe₂. These materials are usually direct-gap semiconductors [1], however previous research has shown that in the lower dimension (1D) transition metal dichalcogenides present metallic character [2]. We present theoretical calculations on 1D transition metal dichalcogenide nanoribbons of various widths (Mo-, W-, S₂, Se₂). We use the open-source Density-Functional-Theory (DFT) package GPAW [3]. We study the electronic properties such as the electron density of states, the band structures and the wavefunctions of these materials. For each material, we consider various terminations of the zig-zag edge with different numbers of chalcogen adatoms. We compare the electronic properties of the quasi 1D structures to the 2D materials and we find that similarly to the 1D MoS₂ nanoribbon, all other structures present metallic character around the edges at the HOMO and LUMO states. Finally, we calculate the edge energy as a function of the chalcogen chemical potential and we conclude on the most stable structure in respect to the number of adatoms.

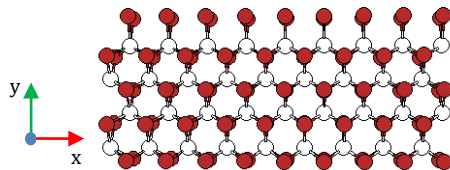


Figure 1: Ball and stick model of a typical MX₂ nanoribbon with two chalcogen adatoms at the zig-zag edge.

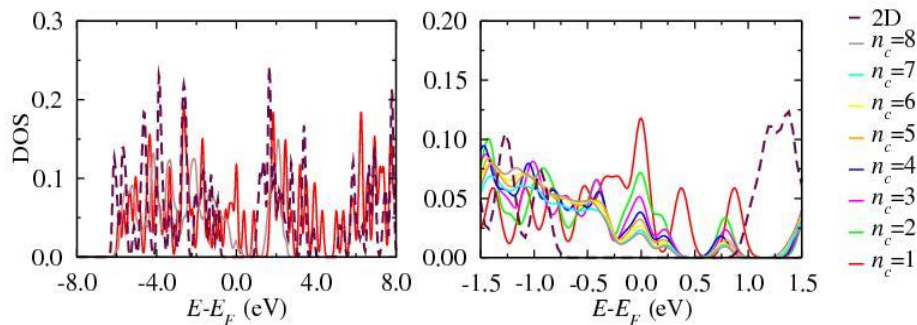


Figure 2: **(Left)** Comparison of electronic DOS between nanoribbons with different widths and the 2D material. **(Right)** Zoomed DOS for all structures around the Fermi level (set at zero eV). In both figures different colours represent different structures (see the legends at the right).

References

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