First Principles Approach to Study Topologically Protected Edge States in 1T′ MoS_2 Nanoribbons

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***Abstract*—The use of novel materials with advanced properties is mandatory to improve device performance and continue scaling for high performance applications at reduced power. Here, we present a first principles approach to evaluate highly conductive topologically protected edge states in 1T′ MoS_2 nanoribbons suitable for carrying large on-currents.**

Keywords- density functional calculations; edge states; topological insulators; nanoribbons

I. INTRODUCTION

First principles calculations predict that well-known two-dimensional materials (MoS_2, $MoSe_2$. WS_2, WSe_2) can exist in topologically nontrivial phases [1,2]. A **k·p** model Hamiltonian whose parameters were fitted to the bulk dispersion relations was used to predict the behavior of the topologically protected edge modes in nanoribbons [2,3]. Due to the interaction between the topologically protected states from the opposite edges [2-4] in a narrow nanoribbon, a small gap in the otherwise gapless linear spectrum of the edge states is predicted to open, resulting in a decrease of the ballistic conductance [2,3]. The gap increases with the magnitude of an orthogonal electric field, resulting in further reduction of the conductance, while the separation between the bulk bands decreases. The edge-localized modes transform into bulk-like modes at a critical value of the orthogonal field, signifying a transition from a topological insulator to a trivial one. As there are no states protected from backscattering, the conductance decreases dramatically [4]. Here, we outline the use of density functional theory to calculate the electronic structure of 1T′ MoS_2 nanoribbons and compare it to the **k·p** approach.

II. METHOD

Predictions regarding the edge states in nanoribbons were obtained within a **k·p** approach. Although accurately calibrated to the first principle bulk dispersion, the approach ignores the peculiarities of the microscopic structures of the edges which, by analogy to graphene edges, may appear in various flavors by cleaving a sheet of two-dimensional materials along different orientations (Fig.1) and by terminating the bonds in different ways. In addition, structural relaxation often results in a reconstructed edge with distinct properties, which is completely ignored within the **k·p** approach. To calibrate our density functional calculations (DFT), we begin by evaluating the bulk band structure of a two-dimensional MoS_2 sheet in the 1T′ phase (Fig. 2). We use the VASP package with the Perdew-Burke-Ernzerhof exchange-correlation functional. We assume a 2 nm vacuum along the OZ-axis and solve the equations on a 12×12×1 *K*-point mesh with a plane wave cut-off of 280 eV. The fundamental band gap of 0.1 eV [1] is reproduced (see Fig. 2). To demonstrate the method's functionality for confined systems, the subband structure of an 8 nm wide nanoribbon cleaved along the OX axis is shown in Fig. 3. Topologically protected edge states with an almost linear dispersion are clearly seen at energies around zero. Surprisingly, no band gap opening in the linear spectrum at zero energy is observed in an 8 nm narrow nanoribbon (Fig. 4), in contrast to **k·p** predictions [2-4]. However, a large band gap of 0.3 eV shown in Fig. 5 is opened after the 2 nm nanoribbon relaxation and optimization. The bandgap in optimized nanoribbons is preserved at other widths as shown in Fig. 6, with the different colors indicating their widths.

III. CONCLUSION

A first principle approach to describe topologically protected states in confined systems is presented. The approach will help to elucidate peculiarities of a topological phase transition in nanoribbons of novel two-dimensional materials using realistic structures.

ACKNOWLEDGMENTS

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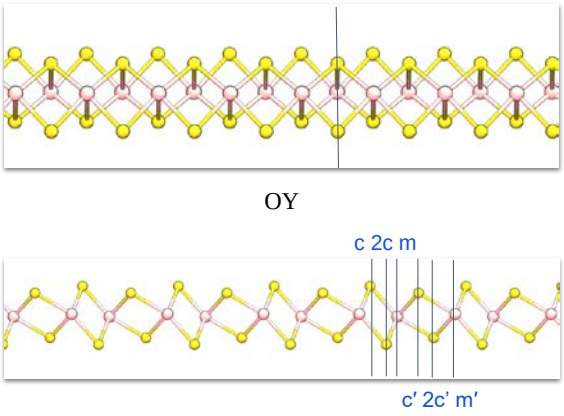

Figure 1. Different egdes of a 1T′ MoS_2 sheet along various planes. In contrast to a nanoribbon confined in the OY direction, six different edges are possible for a nanoribbon confined along OX axis.

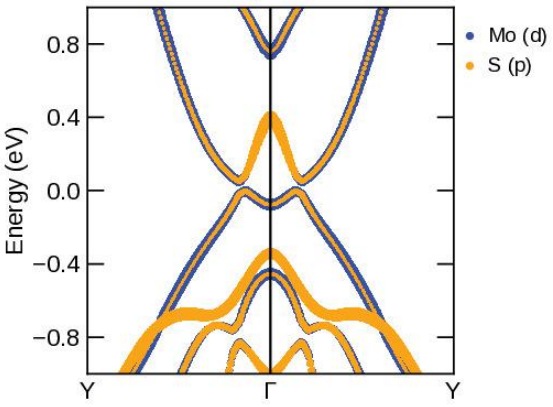

Figure 2. Bulk bands at $k_x = 0$ as a function of k_y in 1T′ MoS_2.

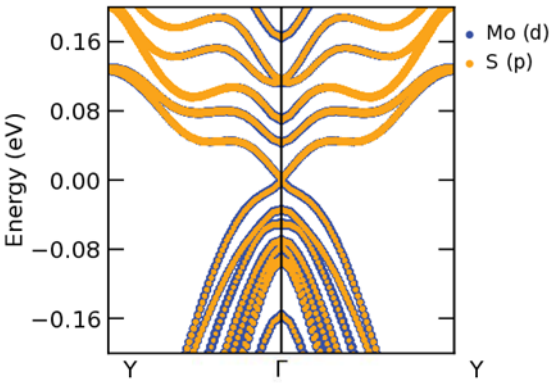

Figure 3. Subbands in an 8nm wide nanoribbon cleaved along *c* edges. Topologically protected edge states with an almost linear dispersion are clearly seen.

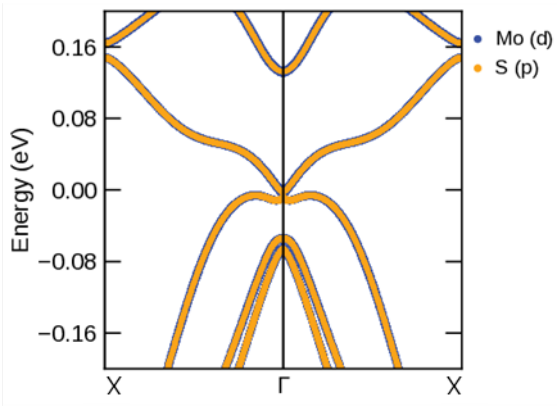

Figure 4. Subband structure in an 8 nm wide (along OY) nanoribbon. The structure is not optimized. In contrast to **k·p** predictions, the band gap does not open for the topological edge state.

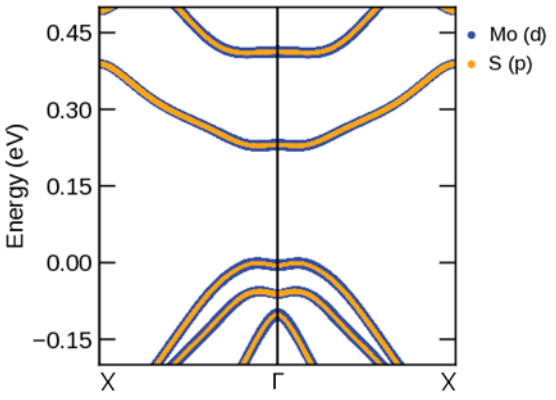

Figure 5. Subbands in a 2 nm nanoribbon along OY after optimization.

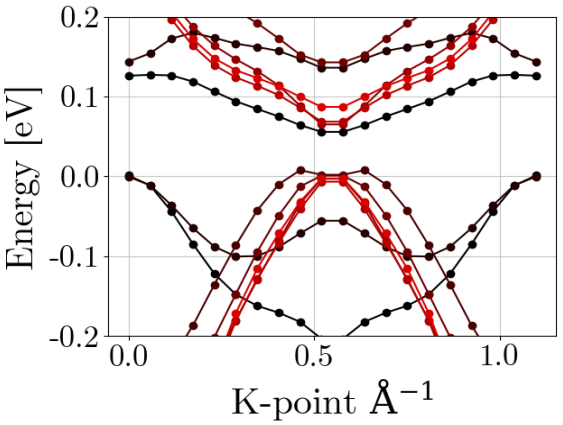

Figure 6. The band gap in the spectrum of the edge states, for several nanoribbon widths along the OY direction. The different colors correspond to different widths from 4 (black) to 12 (red) unit cells (unit cell is equal to 0.32nm).