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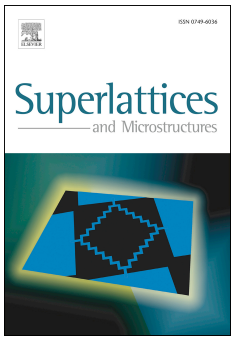


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# Electronic and magnetic properties of $MoSe_2$ armchair nanoribbons controlled by the different edge structures

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## Abstract

Tow-dimensional materials obviously have potential applications in next-generation nanodevices because of their extraordinary physical and chemical properties and the demands of the market. Using first-principle calculation based on density functional theory, we explore electronic and magnetic properties of the different nanoribbons with various edge structures, namely, with hydrogenation or not. In addition, we also calculate the binding energy to analyze the stability of the nanoribbon. Our calculations tell us that the passivated nanoribbons have the positive binding energies, which indicates the passivated nanoribbons are relative stable and hydrogenation can improve the stability of the bare nanoribbons due to the reduction of the dangling bonds. Among of them, full hydrogenation has the highest stability. We find all the nanoribbons with full and without hydrogenation are nonmagnetic semiconductors. It is worth mentioning that hydrogenation can induce the bare nanoribbons to transform gradually from indirect band gap semiconductor to direct band gap semiconductor, even to half-metal. In addition, the magnetic moment of the bare nanoribbon change bit by bit as the rate of hydrogenation increases. When the edge atoms are fully hydrogenated, the magnetic moment return to zero. What's more, our research results still confirm that electronic and magnetic properties of the nanorribons without and with different edge passivation are mainly contributed by the atoms at the edges. These studies about $MoSe_2$ nanoribbons will shed light on the further development of the relevant nanodevices in versatile applications, such as spintronics and energy harvesting.

**Keywords: nanoribbon, transition-metal dichalcogenide, first-principle calculation, hydrogenation, $MoSe_2$**