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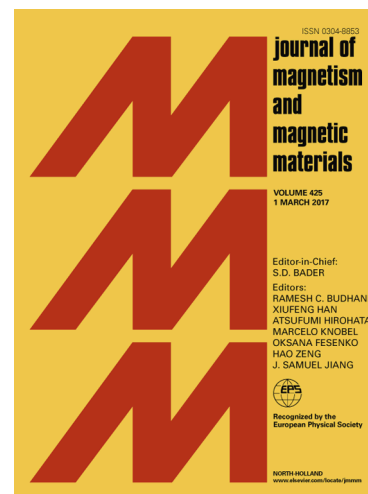
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# Structural and Electronic Properties of PdS<sub>2</sub> Nanoribbons

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## Abstract

First-principles calculations were carried out to predict the stability, electronic, and hydrogen passivation properties of PdS<sub>2</sub> nanoribbons (PdS<sub>2</sub>NRs) with either zigzag- or armchair-terminated edges. Based the energy analysis, we reveal that the armchair NRs are more stable than the zigzag ones. Bare zigzag PdS<sub>2</sub>NRs are metallic, irrespective of the ribbon width. On the other hand, bare armchair NRs change from metal to semiconductor when the ribbon width is greater than 1.24 nm. In addition, different hydrogen passivation type in the armchair direction leads to distinct electronic and magnetic properties of the PdS<sub>2</sub>NRs.

**Keywords:** First-principles, PdS<sub>2</sub>NRs, Hydrogen passivation, Structural properties

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