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Tuning Magnetism of Zirconium Disulfide Nanoribbons by Strain[1] MAHMOUD HAMMOURI, IGOR VASILIEV, New Mexico State University — Monolayer transition metal dichalcogenides have recently attracted considerable attention due to their unusual physical properties and potential applications in nanoscale electronic devices. We carried out *ab initio* density functional calculations to study the electronic and magnetic properties of strained ZrS_2 nanoribbons. Our calculations demonstrated that ZrS_2 nanoribbons without edge passivation were non-magnetic. In contrast, we found that ZrS_2 nanoribbons passivated with hydrogen atoms could switch between the regimes of magnetic and non-magnetic behaviour. Our study showed that edge-passivated armchair ZrS_2 nanoribbons were magnetic under applied strain up to 6%,whereas zigzag ZrS_2 nanoribbons were magnetic under applied strain between 7% and 12%. The results of our calculations suggested the possibility of tuning the magnetism of ZrS_2 nanoribbons by changing the applied strain.

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