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Intrinsic Half-Metallicity in Atomically Thin Zigzag Tungsten Dichalcogenide Nanoribbons[1] PING CUI, University of Science and Technology of China, JIN-HO CHOI, University of Science and Technology of China, Dongguk University-Seoul, JIANG ZENG, ZHENYU LI, CHANGGAN ZENG, University of Science and Technology of China, CHIH-KANG SHIH, University of Texas at Austin, ZHENYU ZHANG, University of Science and Technology of China — Realization of half-metallicity has been serving as a central research emphasis in development of next-generation spintronic devices. To date, only three-dimensional (3D) half-metals have been achieved, while their 2D counterparts remain to be materialized despite of extensive efforts on various predictive designs. This standing challenge is largely due to stringent requirements to establish ferromagnetic order in 2D materials. Here we use first-principles approaches to uncover that atomically thin zigzag tungsten dichalcogenide WX_2 (X = S, Se) nanoribbons stand as the first known intrinsic 2D half-metallic systems, without the typical approach of invoking an external electric field, chemical modification, or carrier doping. The readily accessible half-metallicity is attributed to distinctly different structural reconstructions along the two edges, insulating along one edge, metallic along the other, the latter characterized by the propagation of a robust spin-polarized electron transmission channel. These findings are expected to offer unprecedented opportunities in spintronics purely based on 2D materials.

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