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Distinct Reconstruction Patterns and Spin-Resolved Electronic States along the Zigzag Edges of Transition Metal Dichalcogenides[1] PING CUI, JIN-HO CHOI, WEI CHEN, JIANG ZENG, University of Science and Technology of China, CHENDONG ZHANG, CHIH-KANG SHIH, University of Texas at Austin, ZHENYU LI, ZHENYU ZHANG, University of Science and Technology of China — Two-dimensional transition metal dichalcogenides are a new class of materials exhibiting various intriguing physical, chemical, and mechanical properties. Integration of such materials for potential device applications will necessarily encounter creation of different boundaries. Using first-principles approaches, here we investigate the structural, electronic, and magnetic properties along two inequivalent M- or X-terminated zigzag edges of MX_2 (M=Mo, W; X=S, Se). Along the M-terminated edges, we discover a previously unrecognized but energetically strongly preferred (2x1) reconstruction pattern, which is universal for all the MX_2, characterized by place exchanges of the outmost X and M edge atoms. In contrast, the X-terminated edges undergo a more moderate (2x1) or (3x1) reconstruction for MoX_2 or WX_2, respectively. We further use the prototypical examples of zigzag MoX_2 nanoribbons to demonstrate that the M- and X-terminated edges possess distinctly different electronic and magnetic properties, which can be exploited for a broad range of spintronic and catalytic applications

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Ping Cui
University of Science and Technology of China

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