

Abstract Submitted  
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**First-principles Study of Size and Edge Dependent Properties of MXene Nanoribbons**<sup>1</sup> LIANG HONG, ROBERT KLIE, SERDAR OGUT, Univ of Illinois - Chicago — One-dimensional nanoribbons can be created with considerably different physical properties from their two-dimensional (2D) counterparts due to quantum confinement and surface effects. MXenes are a new class of 2D materials with many potential applications and have drawn significant attention. We perform first-principles calculations to explore the size and edge dependent properties of a wide range of MXene nanoribbons cut from 2D semiconducting MXenes. Our results suggest that semiconducting versus metallic nature as well as the size of the band gap for semiconducting MXene nanoribbons can be tuned as a function of size, chemical composition, and functional groups, which can be useful for future designs of MXene nanostructures with interesting electronic and optical properties.

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