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Structural Stability and Electronic Properties of Two Dimensional Transition Metal Carbides JINYING WANG, ATSUSHI OSHIYAMA, The University of Tokyo — Numerous two dimensional (2D) materials have been developed since the discovery of graphene. High-quality 2D ultrathin Mo₂C films have been successfully fabricated recently [1], but little research on their properties is reported. In this study, we have investigated the structural stability and electronic properties of 2D transition metal carbides (TMC) using first-principles calculations. The pressure of hydrogen are found to be very important for the thickness and surface structure of TMC. The electronic properties of TMC are indicated to strongly dependent on number of d electrons. Nearly all systems are metallic except one. Meanwhile, strain-induced transition between metallic and semi-metallic states have also been found. [1] Xu, C.; Wang, L.; Liu, Z.; Chen, L.; Guo, J.; Kang, N.; Ma, X.-L.; Cheng, H.-M.; Ren, W., Large-area high-quality 2D ultrathin Mo₂C superconducting crystals. *Nat Mater* 2015, 14 (11), 1135-1141.

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