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Intrinsic Magnetism of Grain Boundaries in Two-dimensional Metal Dichalcogenides ZHUHUA ZHANG, XIAOLONG ZOU, Department of Mechanical Engineering and Materials Science, Rice University, Houston, VINCENT H. CRESPI, Department of Physics and Materials Research Institute, The Pennsylvania State University, University Park, Pennsylvania, BORIS I. YAKOBSON, Department of Mechanical Engineering and Materials Science, Rice University, Houston — In two-dimensional (2D) atomic crystals, ubiquitous grain boundaries (GBs) have been shown to cause considerable degradation in material properties. Using first-principles calculations, we show that dislocations and GBs in 2D metal dichalcogenides MX_2 (M=Mo,W; X=S,Se) exceptionally exhibit substantial magnetism, in sharp contrast to other 2D materials. All dislocations are shown to have a high magnetic moment of 1.0 Bohr magneton, mainly contributed by the Mo 4d orbitals. GB composed of pentagon-heptagon pairs shows ferromagnetic spin ordering and undergoes transitions from semiconductor to half-metal and to metal as tilt angle increases; when the tilt angle is over 47°, GB prefers square-octagon pairs and turns to antiferromagnetic semiconductor. A novel mechanism based on interplay between dislocation-induced localized states and local unbalanced stoichiometry of GB is revealed for elucidating the magnetic behavior. Our findings suggest that purposeful engineering of topological GBs can upgrade 2D MX_2 into promising magnetic semiconductors for spintronic applications.

Zhuhua Zhang
Department of Mechanical Engineering and Materials Science,
Rice University, Houston

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