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Magnetic Proximity-Induced Colossal Valley Splitting in WTe_2 for Room Temperature Valleytronics

Ahsiur Rahman Nirjhar and Saquib Ahmed*

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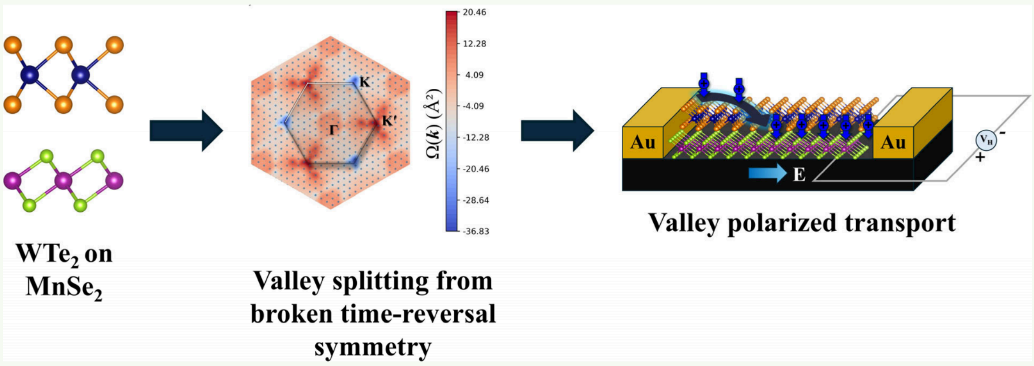

ABSTRACT: Valleytronics, a burgeoning field of information technology, offers exciting possibilities for future information storage and computing. However, fully realizing its potential hinges on overcoming the inherent valley degeneracy in valleytronic materials. This study explores the possibility of lifting valley degeneracy in monolayer 2H-WTe_2 by using $MnSe_2$, a room-temperature ferromagnet, as a substrate. First-principles calculations show that a significant valley splitting of 236 meV can be achieved in the $WTe_2/MnSe_2$ heterostructure. This high level of splitting is attributed to the short-range magnetic proximity effect, mediated by interfacial orbital hybridization due to spatial charge redistribution and manifested by the induced magnetic moment on the W atom. The Berry curvature calculation confirms the broken time-reversal symmetry responsible for lifting the valley degeneracy, and the valley splitting can be further enhanced by modulating the interlayer distance. The Curie temperature of the $MnSe_2$ substrate is estimated to reach 457.57 K with 6% biaxial tensile strain, with the valley splitting retaining a value of 191 meV at this strain. The heterostructure also exhibits suitable band alignment for valley-polarized carrier transport and realization of the anomalous valley Hall effect, where the valley and spin indices of the carriers can be controlled by switching the magnetization direction of the $MnSe_2$ substrate. These phenomena, along with the strain tolerance of valley splitting, present a promising path toward room-temperature valleytronics, potentially revolutionizing future information technologies.

KEYWORDS: *valley splitting, valleytronics, magnetic proximity effect, 2H-WTe_2, TMDC, heterostructure, 2D magnetic material*

INTRODUCTION

Following the discovery of graphene, two-dimensional (2D) materials, including transition-metal dichalcogenides (TMDCs), MXenes, MBenes, and other 2D compounds have attracted considerable interest due to their distinct and nonubiquitous properties, offering the potential for a wide array of novel applications.[1−6] Among these materials, the multivalley electronic structure of TMDCs and some other 2D materials stand out as particularly intriguing. In contrast to traditional semiconductors, which include the conduction band minimum (CBM) or valence band maximum (VBM) at a singular position in the Brillouin zone, these materials possess these energy extrema at several equivalent places, referred to as valleys.[7−10] TMDCs are direct-band-gap materials, with the VBM and CBM located at the corners of the Brillouin zone. The noncentrosymmetric D_{3h} crystal symmetry forms two inequivalent valleys at the K and K' points.[11,12] The valley index of the carriers functions as an additional degree of freedom akin to charge and spin. Various valley-related phenomena, such as valley-dependent circular dichroism,[13] valley-polarized electroluminescence,[14] the valley-Hall effect,[15] and the valley-Zeeman effect,[16] have already been experimentally demonstrated. Controlling and manipulating the charge and spin degrees of freedom have led to advancements in electronics and spintronics. The valley degree of freedom establishes a foundation for valleytronics, a promising domain

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