SEMINAR ANNOUNCEMENT

國立中山大學物理系112學年度第二學期專題演講

High Thermoelectric Performance in 2D Technetium Dichalcogenides TcX_2 (X = S, Se, or Te)

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Abstract

In recent years, the search for alternative energy sources has been of major research interest, and one of the potential solutions is thermoelectricity. Moreover, studies on the emergence of transition-metal dichalcogenides (TMDs) have been unstoppable because of their unique properties. Among this group of materials, technetium-based TMDs (TcX_2, where X = S, Se, or Te) are one of the least investigated materials. Using first-principles calculations, we systematically studied the structural stability and electronic properties of bulk and monolayer TcX_2 in $1T^{dp}$ (1T double prime), 1T′, 1T, and 2H crystal structures as well as the thermoelectric properties of the bulk and monolayer $1T^{dp}$ phases. Formation energy calculations, phonon dispersion, and molecular dynamic simulation results revealed that only the $1T^{dp}$ phase is stable, while 1T′, 1T, and 2H are unstable. These findings imply the possible synthesis of monolayer $1T^{dp}$-TcX_2. With regard to the electronic properties under the hybrid functional approach, bulk $1T^{dp}$-$TcTe_2$, $TcSe_2$, and TcS_2 exhibit indirect band gaps of 0.37, 1.01, and 1.19 eV, respectively. For the monolayer phase, enlarged indirect band gaps of 1.21, 1.64, and 1.87 eV, respectively, were observed. Surprisingly, the calculated ZT numbers at 1200 K for monolayer $TcTe_2$ are 1.78 (p-type) and 1.84 (n-type), which are comparable to those of the currently synthesized excellent thermoelectric materials. Finally, the thermoelectric properties of $TcTe_2$ are significantly improved when reducing the dimensionality from bulk to monolayer at high temperatures. Our findings provide crucial evidence regarding the structural stability, robust electronic properties, and excellent thermoelectric properties in TcX_2 for potential optoelectronic and thermoelectric applications.

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