Continuous phase transition of the MoS_2 from 2H to 1T' state by using 2D electride: Ca_2N

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Abstract

The lattice engineering of the sulfide based transition metal dichalcogenide (TMDs) is difficult compared to selenide and telluride materials.[1] Here, we report on the continuous phase transition of the few layers to bulk molybdenum disulfide (MoS_2) system by realizing the hetero-structures with the low work function (2.6 eV) two dimensional electride (2D-$[Ca_2N]^{+}\cdot e^{-}$) that contain highly mobile electrons[2], where the large work function differences (>2 eV) between them is the key of the degenerate electrons doping that is distributed over a distance of few tens of nanometer from the contact interface in contrast to the other surface limited (~1 nm) chemical functionalizations or ionic gating approaches.[3] An electron doping density of ~10^{14} cm^{-2} was estimated on the MoS_2 layers that performed exceptional layer thickness dependent lattice symmetry change from the 2H to 1T' phases until a few-layer (~10 nm) and then strong doping effect to the bulk samples resulting a giant band gap re-normalization by ~200 meV along with the softening of the commonly observed Raman modes by the $\Delta\omega$=10 cm^{-1}. As the MoS_2 thickness was decreased, well defined Raman peaks of 2H crystal were gradually disappearing along with the emergence of other 1T' phase Raman modes, thus elucidating the symmetry change feature due to concentrated charge density in a thinner film. Additionally, a hetero-structure of the few-layer MoS_2 demonstrated multiple in-plane anisotropic Raman modes, including those of metallic phases Raman modes along with the presence of the hugely shrunk (250 meV) optical gap and enhanced PL intensity than a pristine monolayer MoS_2; a realization of the few-layer 2H-MoS_2 crystal with distorted symmetry and direct band gap structure when placed on the top of the $[Ca_2N]^{+}\cdot e^{-}$. This is attributed to the long-range electron doping induced structural change across the K-Γ line, hence provided an opportunity to discover various kinds of 2D materials using a single 2D-dopant suitable for the future optoelectronic application.

KEYWORDS: MoS_2, electride, doping, long range, phase-transition, direct band gap structure

References

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