

Supplementary Materials for

K- Λ crossover transition in the conduction band of monolayer MoS₂ under hydrostatic pressure

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The pressure rate of the in-plane lattice constant of Si can be calculated to be about 1.02%/GPa according to its Young's Modulus (45). Assuming that the pressure rate of the in-plane lattice constant of monolayer MoS₂ to be about 0.24%/GPa, the same as that of bulk MoS₂ (46), we can conclude that the extra strain in plane should be compressive strain. So it is possible to induce an additional compressive strain to monolayer MoS₂ by Si/SiO₂ substrate.

In order to investigate this, we measured the Raman spectra of monolayer MoS₂ under various pressures and plotted them in the following figures:

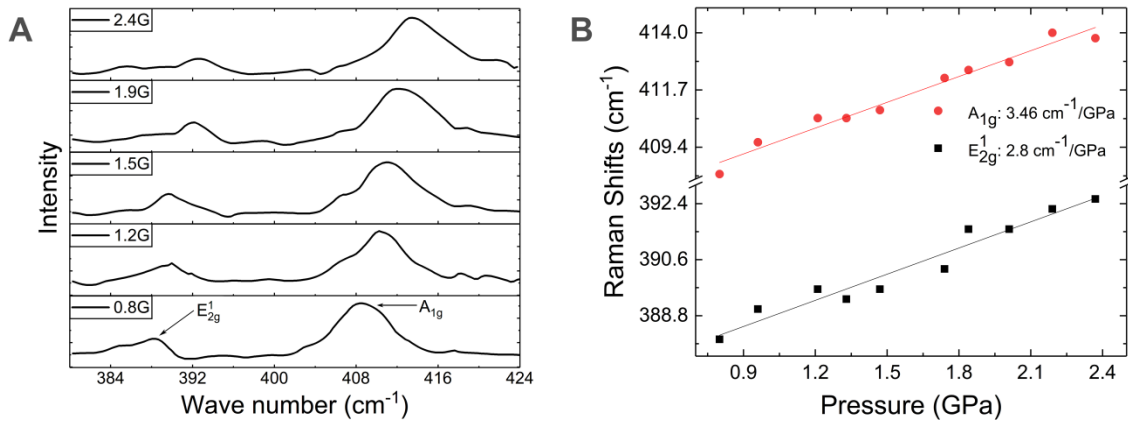


fig. S1. Raman spectra of monolayer MoS₂ under various pressures. (A) Raman spectra of monolayer MoS₂ under 0.8 GPa, 1.2 GPa, 1.5 GPa, 1.9 GPa, 2.4 GPa. (B) Raman shifts of monolayer MoS₂ versus pressure. With pressure increasing, the in-plane mode of E_{2g}¹ and out-of-plane mode of A_{1g} blueshift at a rate of 2.8 cm⁻¹/GPa and 3.46 cm⁻¹/GPa, respectively.

We can see that, along with increasing the pressure, the in-plane mode of E_{2g}¹ is slightly smaller than that of the out-of-plane mode of A_{1g}. Thus the additional compressive strain induced by Si/SiO₂ substrate can be neglected. We think that herein the 300 nm amorphous SiO₂, which has the van der Waals interaction with the monolayer MoS₂, plays a buffer layer role that releases the strain transmitted from the Si substrate.