Tuning the Excitonic Response of Monolayer WS_2 Domes via Coupled Pressure and Strain Variation

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In our work [1], we investigated micrometric 1L-WS_2 domes (Fig. 1a), in which the 1L crystal undergoes bi-axial tensile strain at the centre and uniaxial tensile strain at the borders. We manipulated the dome morphology through the application of pressure, to achieve a modulation of these complex strain components, and investigated the sample response by μ-Raman and μ-photoluminescence. We found that, on increasing pressure, the system reduces in volume maintaining a constant basal radius. This pressure-induced distortion of the dome shape determines an increase in the out-of-plane compressive strain, while the in-plane tensile strain remains constant. The non-trivial, coupled evolution of morphology and strain in the 1L-dome leads to an anomalous pressure evolution of the band extremes in the conduction band, responsible for a pronounced non-linearity in both the intensity and energy trend of the exciton under pressure. We found evidence of a hybridization mechanism between distinct conduction band extremes resulting in an exciton emission with mixed direct/indirect nature and in-plane/out-of-plane orbital character; see Fig. 1b.
Our study demonstrates that pressure and morphological strain can be coupled in 2D semiconductors to obtain modulations of the electronic band structure not achievable in planar monolayers.

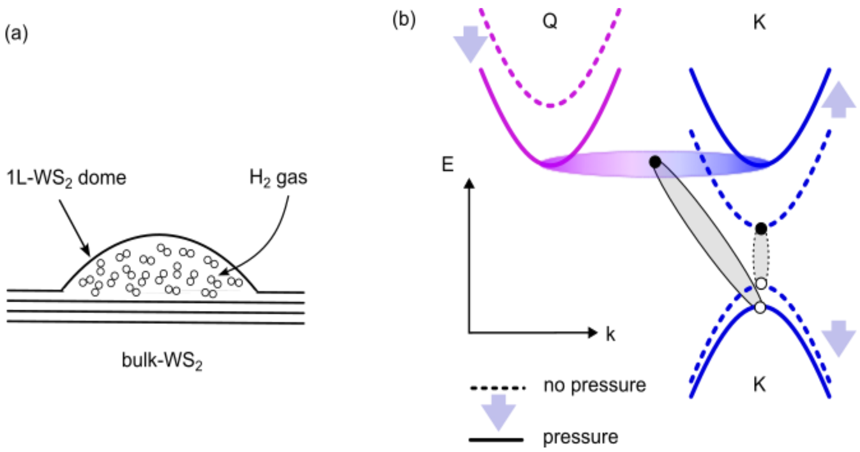

Fig. 1. (a) Graphical representation of a 1L-WS_2 dome. Domes are produced on top of bulk samples by hydrogen ion irradiation: they consist of H_2-filled, hemispherical 1L membranes lifted from the underlying bulk. (b) Scheme of the hybridization mechanism observed under pressure. Dotted lines represent the band structure at ambient conditions, when the exciton recombination occurs at the K point, while continuous lines represent the band structure at high-pressure, when a hybridized exciton is formed by mixing the electronic states at K and Q in the conduction band.

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References

[1] E. Stellino, B. D'Alò, E. Blundo, P. Postorino and A. Polimeni, ,*NanoLetters*, 2024, **24,** 13, 3945–3951.