Electronic Supplementary Material (ESI) for Nanoscale.
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Supplemental Information

Precise and reversible band gap tuning in single-layer $MoSe_2$ by uniaxial strain

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Supporting Information Contents

1. Mono- bilayer spectra

Figure S1(a) shows an optical transmission image of the same flake as described in the main text. The monolayer and bilayer locations of the flake are indicated. The spectra for each region can be seen in Figure S1(b). The monolayer PL intensity is much larger than the bilayer region, as expected.

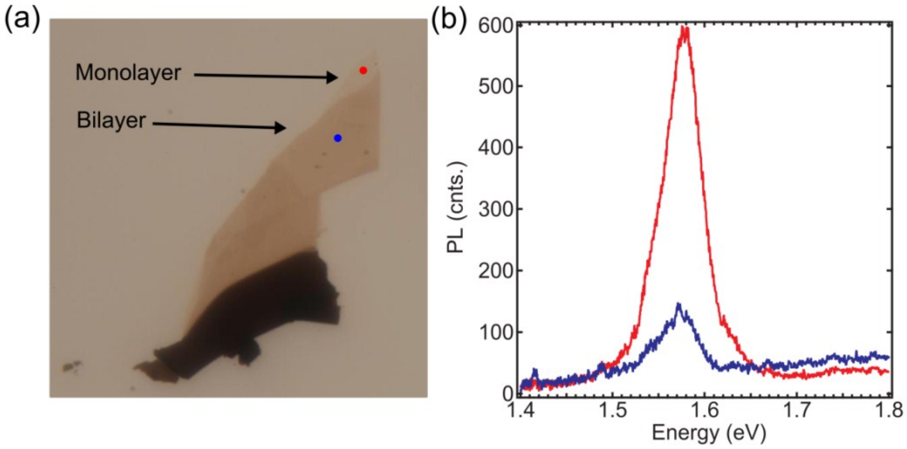

Figure S1: (a) Transmission mode optical image of a $MoSe_2$ flake with single, bilayer, and multilayer regions. (b) PL spectra for the single layer portion in (a) (red dot) and bilayer portion (blue dot).

2. Uniform strain estimation

Strains (ϵ) are calculated given the thickness (t) of the substrate and the radius of curvature (R) of the substrate while strained, $\epsilon = t/2R$. The radius of curvature can be simply estimated given an optical image of the strained substrate, such as those in Figure S2(b-d). For more efficient calculation of the strain, given a simple measureable quantity (the distance between the movable plateaus) we wrote a script that uses the bisection method to calculate the radius of curvature given the chord length (from tip to tip) of the substrate arc. The chord length is measured using calipers to measure the distance between the plateaus (See Figure 1(c) of the main text). Figure S2(e) shows an output plot of this script for a sample substrate with a length of 46.3 mm.

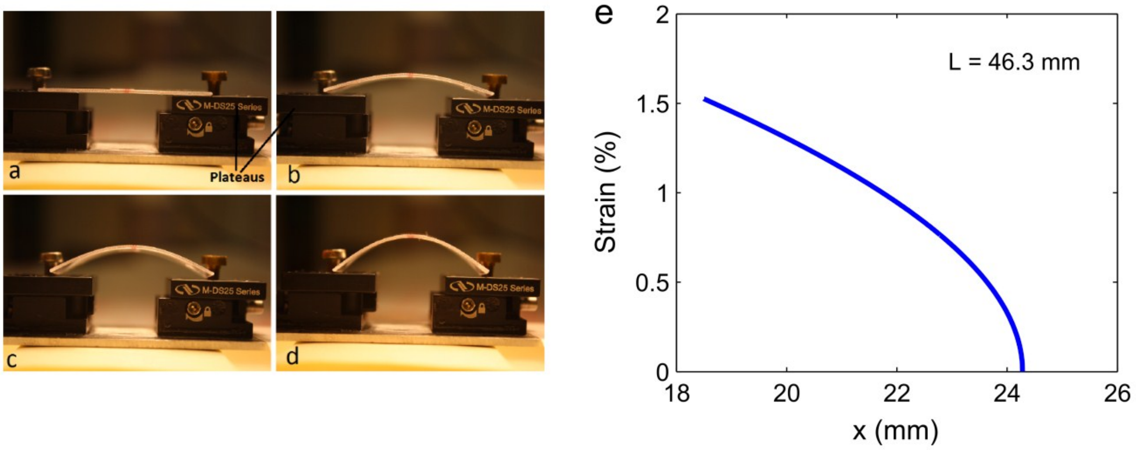

Figure S2: (a-d) Optical images of the bending apparatus for varying strains. Strain estimation for a given distance, x, between the platforms of the bending apparatus.

3. Band gap change with strain (DFT calculations)

Figure S3 shows the calculated band gap (ZORA and with spin-orbit coupling, ZORA + SOC, see Materials and Methods of the main text). For the armchair and zigzag directions the band gap changes by -47 and -48 meV per percent of strain, respectively (black and red curves in Figure S3). For biaxial strain the band gap changes by -87 meV per percent of strain (green curves in Figure S3). When we take into account the Poisson's ratio of the substrate of 0.37 % for 1% strain, the band gap trend is much shallower, showing a band gap change of -32 meV per percent of strain, in agreement with our experimental strain results.

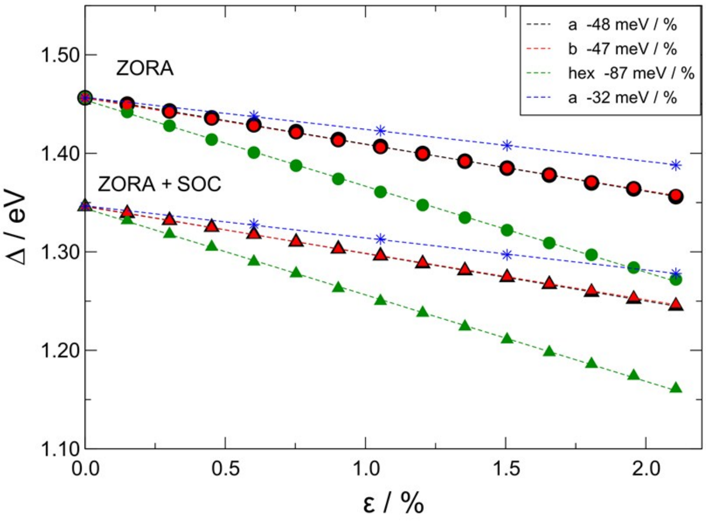

Figure S3: Calculated change in band gap for strain up to ~2%. The red and black curves show the trends for the armchair and zigzag directions. The green curve shows the trends for the biaxial strain. The blue curve shows the trend while taking into account the effect of the substrate (see main text).

4. Strict compression along armchair axis (DFT calculations)

Figure S4 shows the change in band gap for monolayer $MoSe_2$ with compression and strain. Considering the Poisson's ratio of the polycarbonate substrate, we have shown the the change in the band gap is slower than if the strain is completely uniform along one axis (see Figure S3 above). The slower change in band gap is due to the small increase in band gap from compression along the direction perpendicular to the strain axis.

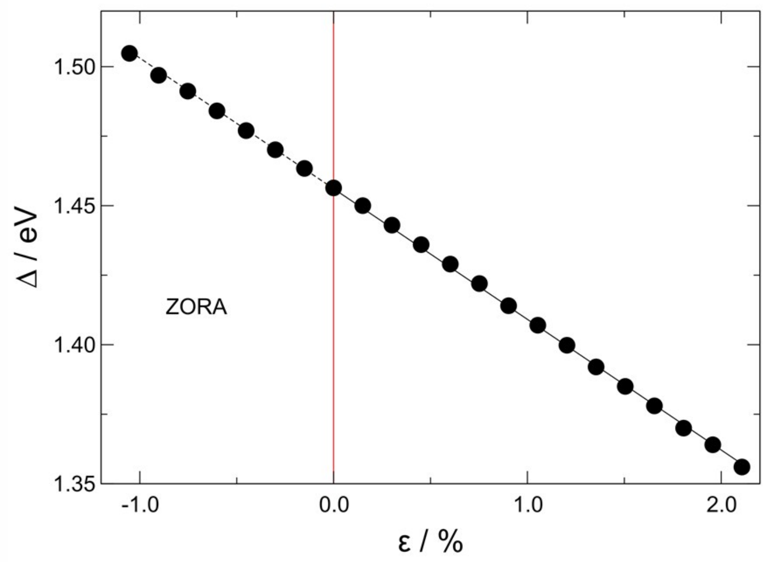

Figure S4: Calculated change in band gap for compression of 1% to a strain of 2% along the armchair direction.