

Supplementary Information

Analysis of Localized Excitons in Strained Monolayer WSe₂ by First Principles Calculations

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Table S1. Exciton energies (in eV) for pristine and wrinkled monolayer WSe₂ by nano-indentation (R=1.5 nm and H= 0.1 nm).

Energy	Dark exciton	X_A	X_A^{2s}	X_B	X_B^{2s}	X_C
Pristine	1.53	1.58	1.90	2.02	2.37	2.82
Wrinkle	1.15	1.30	1.59	1.82	2.39	2.67

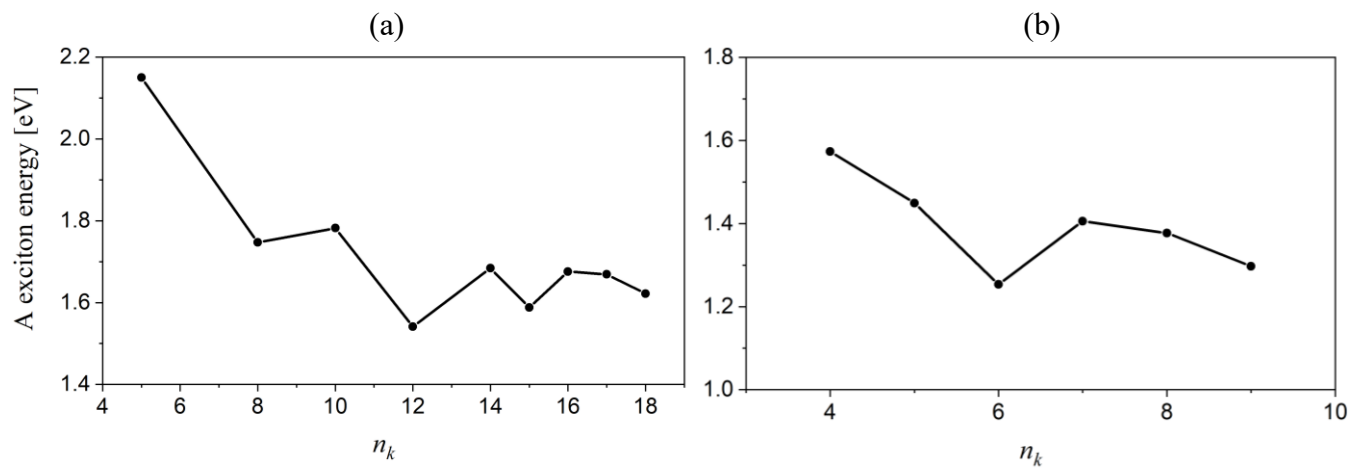


Fig. S1. Calculated A exciton energy (GW-BSE) vs. n_k for (a) $n_k \times n_k \times 1$ k sampling for pristine monolayer WSe₂, and (b) $1 \times n_k \times 1$ k sampling in the GW-BSE for the nano-indented wrinkle (R=1.5 nm and H= 0.1 nm).

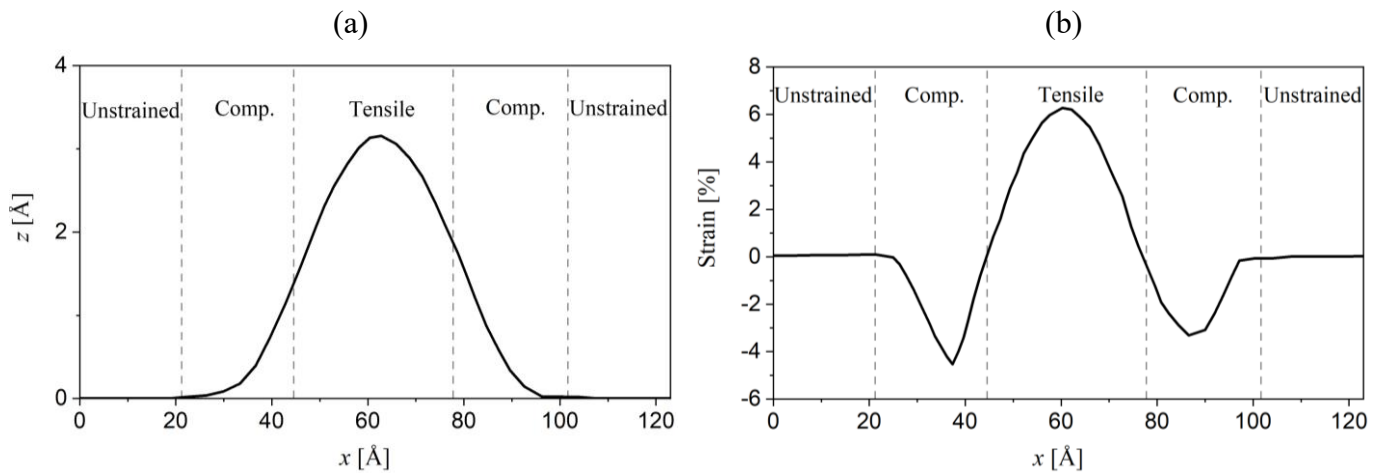


Fig. S2. (a) Height and (b) strain vs. x coordinate in the nano-indented WSe₂ monolayer; $R = 5$ nm and $H = 0.31$ nm.

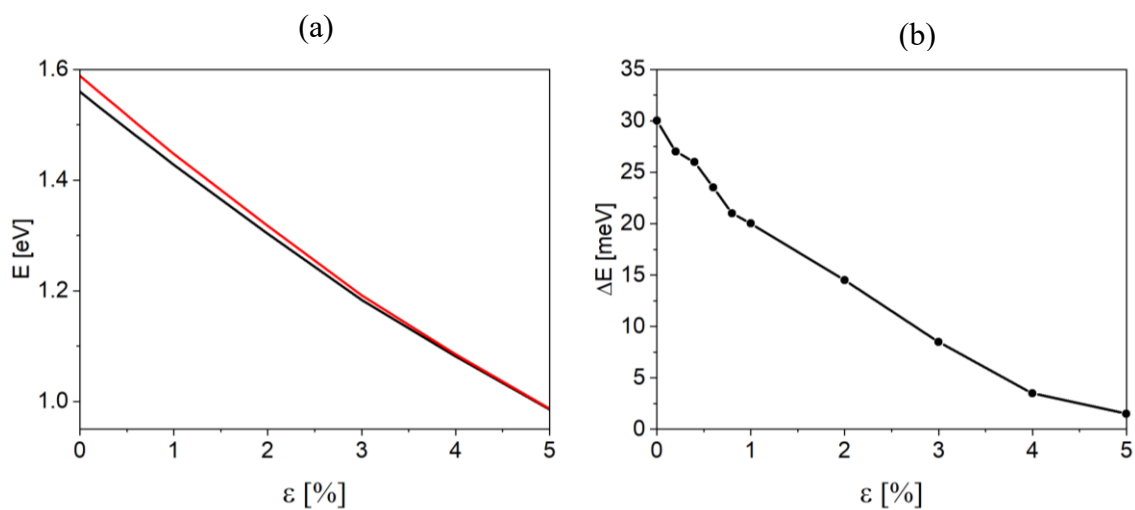


Fig. S3. (a) Exciton energy vs. biaxial strain for the lowest energy dark exciton (black line) and A exciton (red line). (b) Energy difference between the A exciton and the lowest energy dark exciton vs. strain.

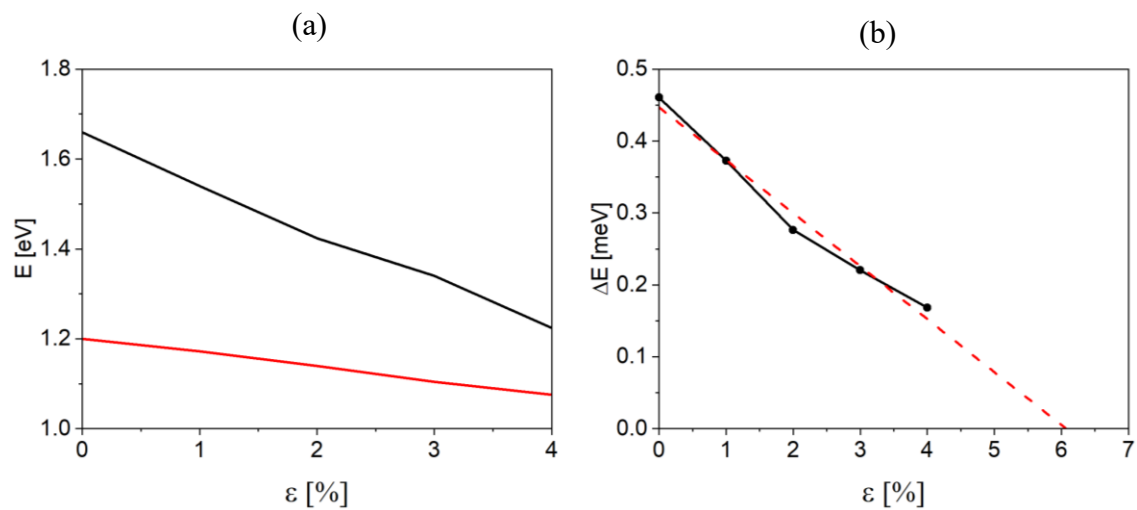


Fig. S4. (a) Exciton energy vs. biaxial strain for the A exciton (black) and the lowest SV exciton (red). (b) Energy difference between the A exciton and the lowest SV exciton vs. strain. Dots indicate the calculated data and the dashed line is a fit.