Abstract Submitted
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Curvature-controlled valley polarization and band-gap tuning in few-layer MoS_2 PEKKA KOSKINEN, NanoScience Center, Department of Physics, University of Jyväskylä, Finland, IOANNA FAMPIOU, ASHWIN RAMASUBRAMANIAM, Department of Mechanical and Industrial Engineering, University of Massachusetts, Amherst — Monolayer transition-metal dichalcogenides (TMDCs) display valley-selective circular dichroism due to time-reversal symmetry and lack of inversion symmetry, making them promising candidates for valleytronics. In contrast, few-layer TMDCs possess both time-reversal and inversion symmetry and hence, lose these desirable valley-selective properties. Here, by using density-functional tight-binding electronic structure simulation and revised periodic boundary conditions, we show that bending of multilayer MoS_2 sheets breaks band degeneracies and localizes states on separate layers due to bending-induced strain-gradients across the sheets. We propose a strategy for employing bending deformations as a simple yet effective means of dynamically and reversibly tuning band gaps while simultaneously tuning coupling between spin, valley, and layer pseudospin of charge carriers in few-layer TMDCs.

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