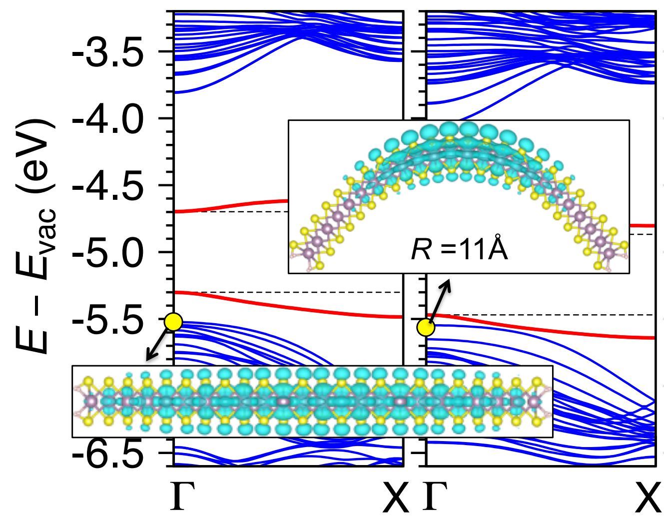
Bending 2D Materials to Control Electrical Conductivity: Key to Clean Energy and Flexible Nanoelectronics



Bending induced charge localization and Fermi-energy level shift in armchair 1H-MoS_2 nanoribbon. The lower red-curve corresponds to the occupied edge states whose energy decreases with increasing bending curvature. The wave functions of top non-edge valence bands get localized to the middle region of the nanoribbon when bending is applied.

L. Yu, A. Ruzsinszky, and J. P. Perdew, *Nano Letters* 16, 2444 (2016)

Work was performed at Temple University

Scientific Achievement

First-principles calculations demonstrate that electrical conductivity can be controlled in some 2D materials by mechanical bending.

Significance and Impact

Opens a new route for designing functional 2D materials for clean energy and nanoelectronic applications (e.g., flexible solar cell, foldable display, skin-like sensor) in which flexuosity is essential.

Research Details

– Bending can induce controllable charge localization in the MoS_2 and phosphorene nanoribbons, whence the electrical conductivity can be altered or turned on and off.

– No sizable bending effects on the electronic properties of graphene are found, making graphene suitable for applications where flexibility without other property change is required.

– The effective thickness of a 2D material is uniquely derived and calculated from first-principles, allowing one to compare the physical properties of interest between 2D and 3D materials.