Calculations on structural, electronic, and energetic properties

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Overview of the tutorial

- Purpose: This section is to familiarize users with calculating some basic properties of materials. These include relaxing a material to obtain the equilibrium structure at 0 temperature, electronic structure (e.g., density of states and band structure) for a given ionic configuration, and energetic properties of different phases.
- Approaches: SCAN meta-GGA
- Codes: VASP
- Materials: Si

Running SCAN in VASP

INCAR tags:

METAGGA = SCAN

LASPH = .TRUE.

ADDGRID = .TRUE.

POTCAR:

Check if it contains the kinetic energy density of the core electrons:

grep kinetic POTCAR

Note on Band-structure and DOS calculations

- self-consistent vs. non-self-consistent
- For non-scfconsistent:
  - Need converged charge-density and kinetic energy density
  - Kinetic energy density is not written out after calculation.

four examples

- Si
  - Lattice constant, band structure
  - Phase transition
  - Defect formation energy

- MoS_2
  - Lattice constant, band structure, DOS
    - Non-selfconsistent, "incorrect"

Unusual Mechanical and Electronic Properties of 2D Materials Predicted by Using SCAN

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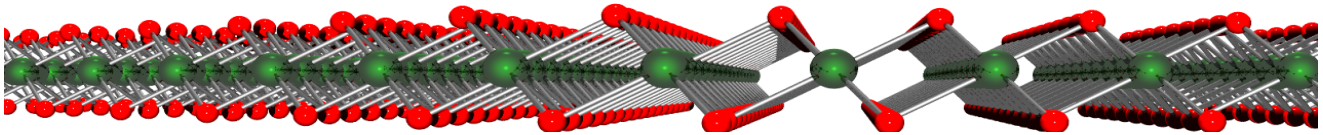
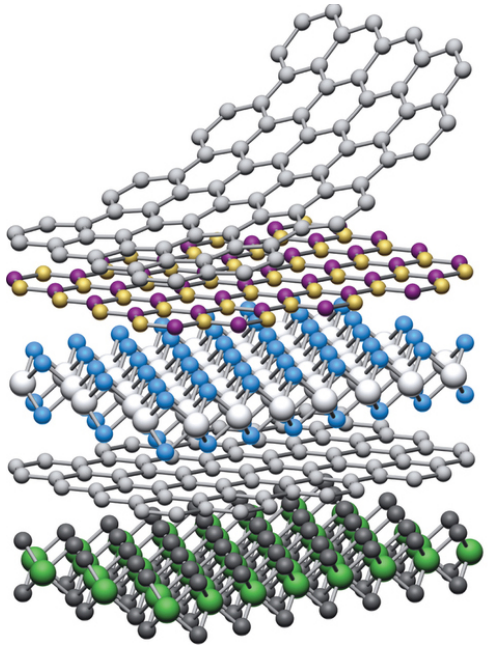
Collaborators:
Qimin Yan, Adrien Ruzsinszky, John Perdew

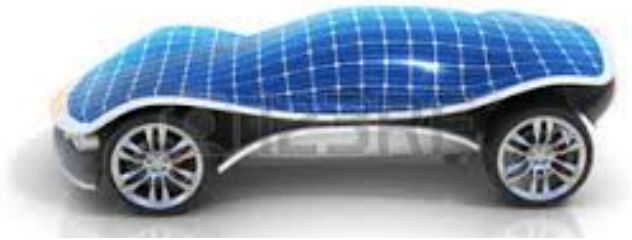
Center for the Computational Design of Functional Layered Materials

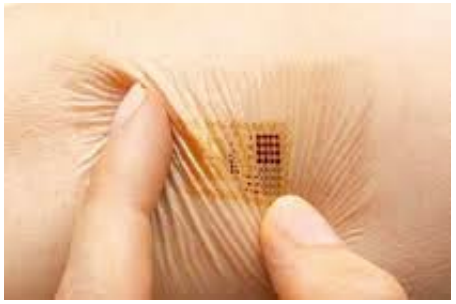


Unique Attributes of 2D Materials

- van der Waals interlayer bonding
  - Artificial heterostructures
  - New functionalities
- Atomically thin & highly flexible
  - Flexible and large-area electronics



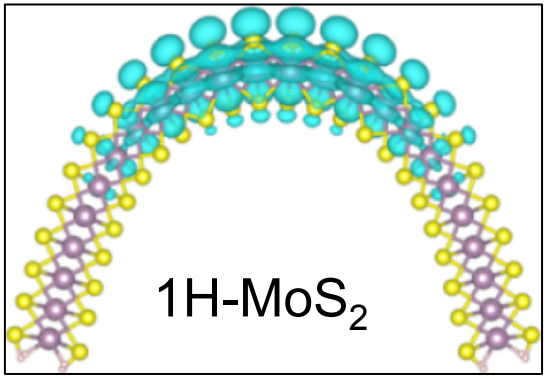




Two examples

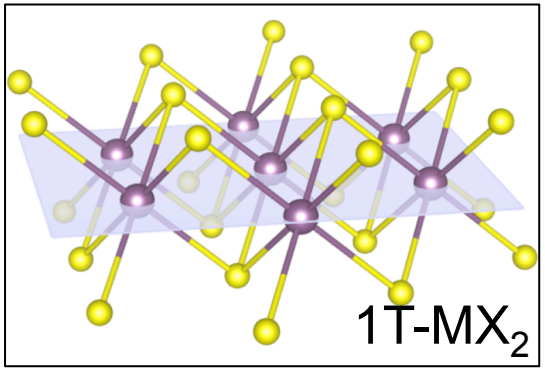
- Extraordinary 2D bending effects
  - Yu, Ruzsinszky & Perdew

    Nano Letters, 16, 2444(2016)

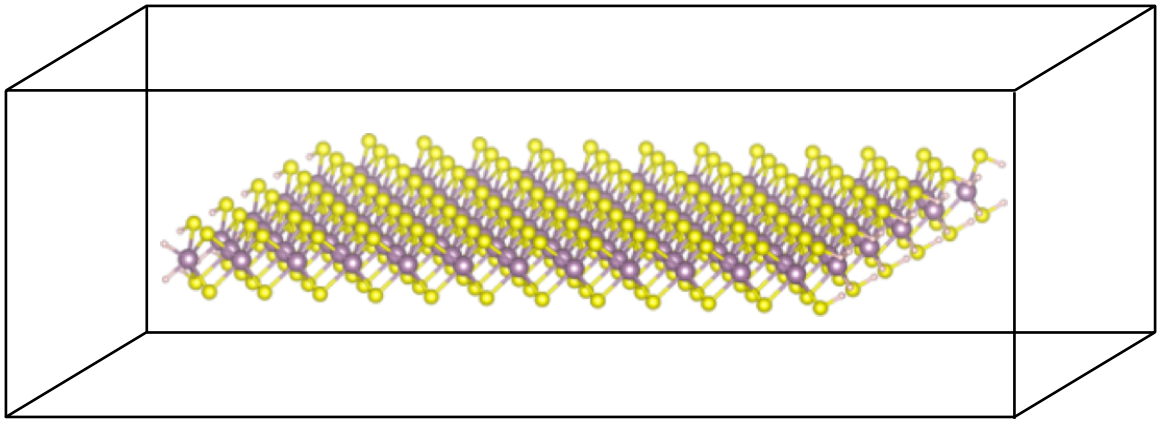


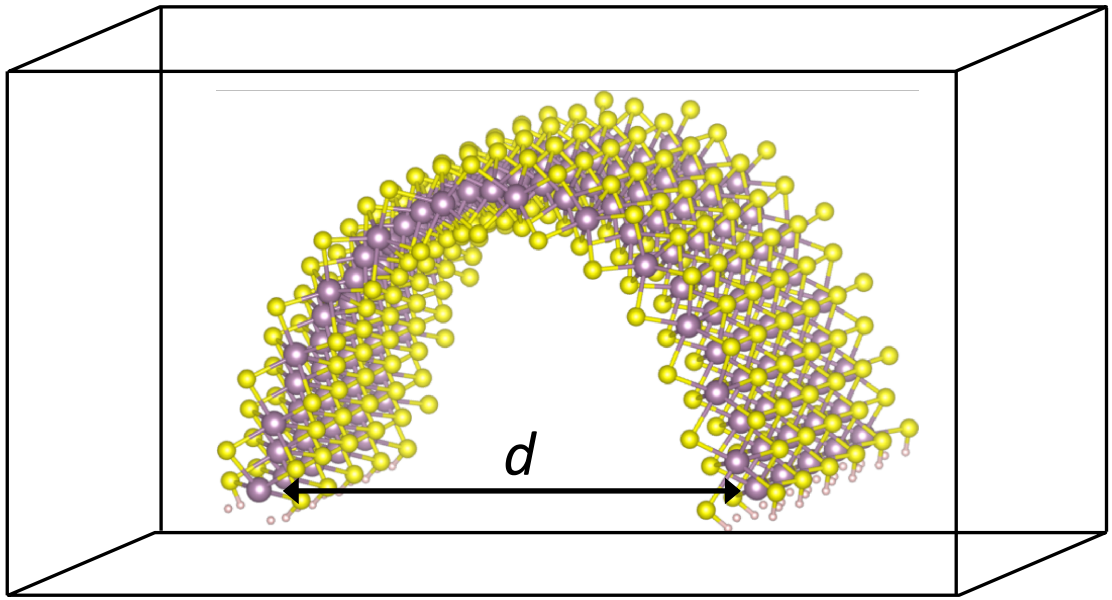
- Counter-intuitive auxetic effects in 1T MX_2
  - Yu, Yan & Ruzsinszky,

    Nat. Communs. 8, 15224 (2017).



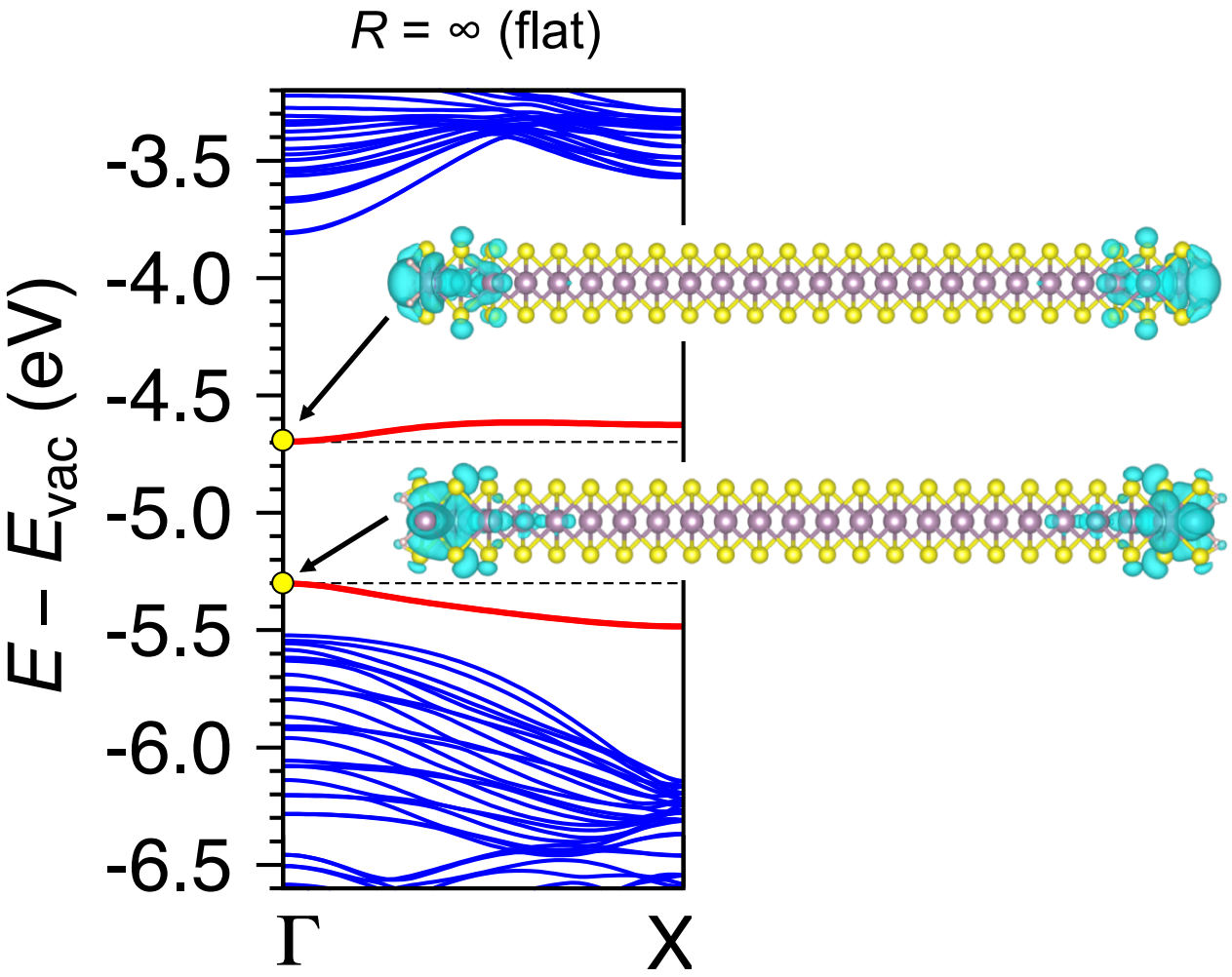
Bending Scheme: Case of MoS_2 Nanoribbon





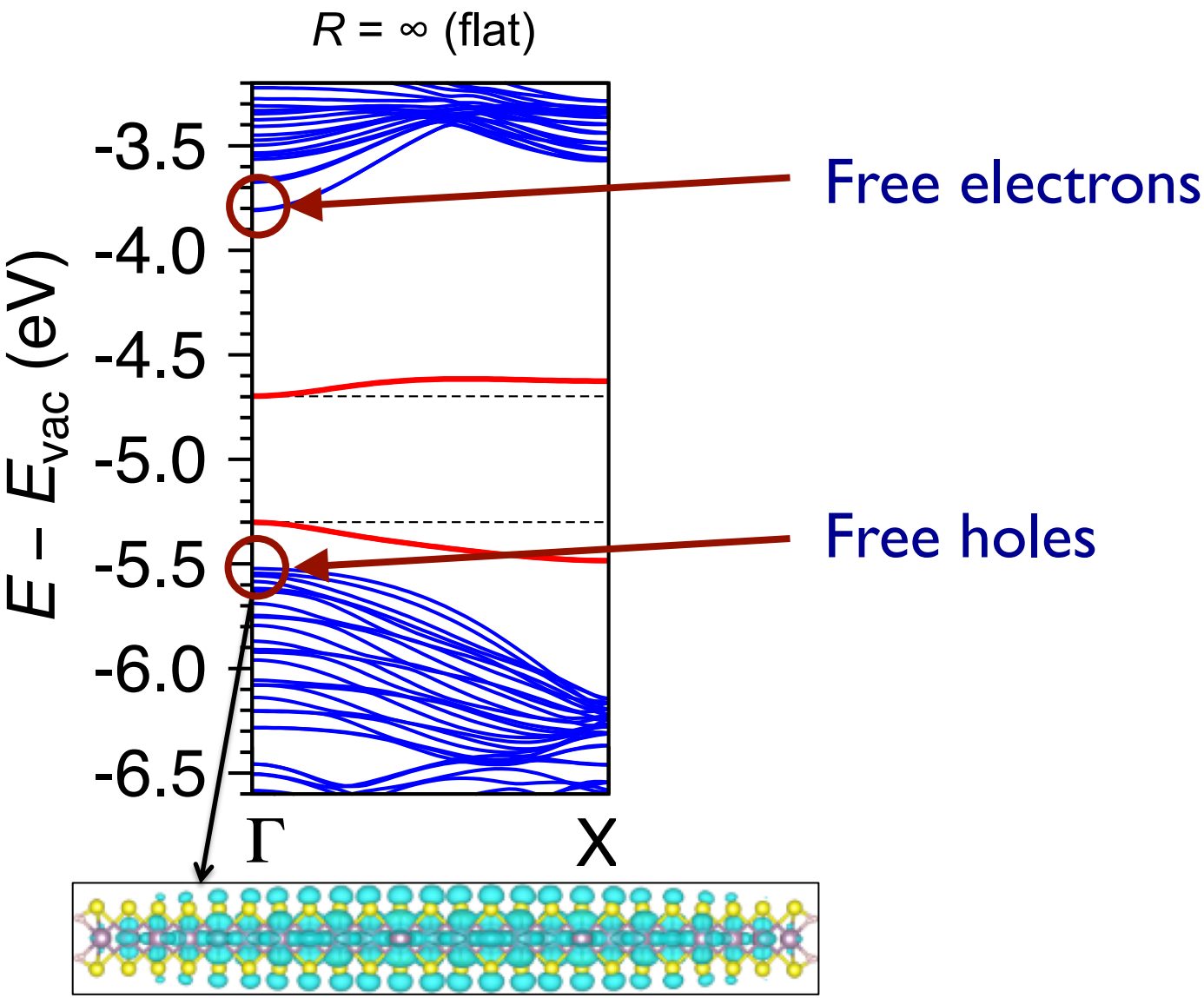
Similar to the set-up for 2-point bending stiffness measurement

Band Structure of Armchair MoS_2 Nanoribbon

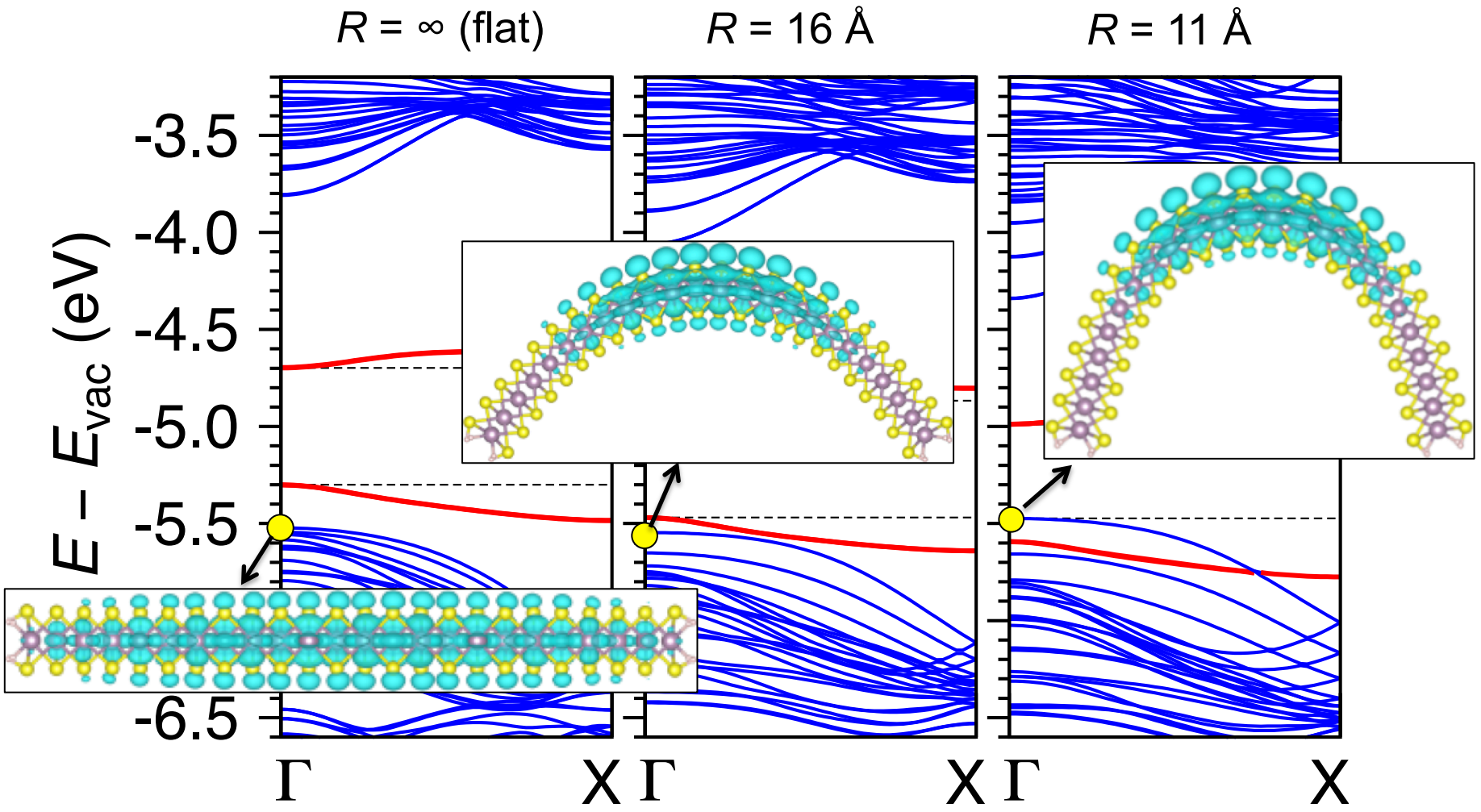


L. Yu, A. Ruzsinszky, J. Perdew, Nano Letters, 16, 2444 (2016)

Free Carriers in MoS_2 Semiconductors



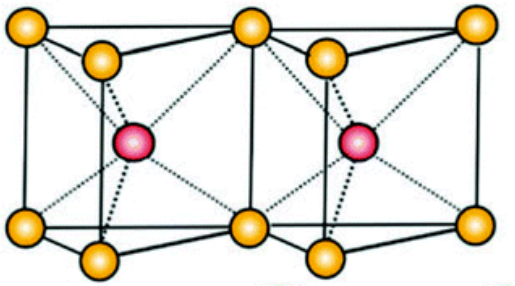
Bending Localizes Hole Carriers in MoS_2



- Bending switches on/off p-type conductivity

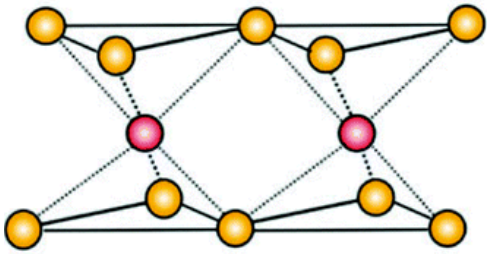
Monolayer MX_2: 2H vs. 1T

2H
triangular
prismatic



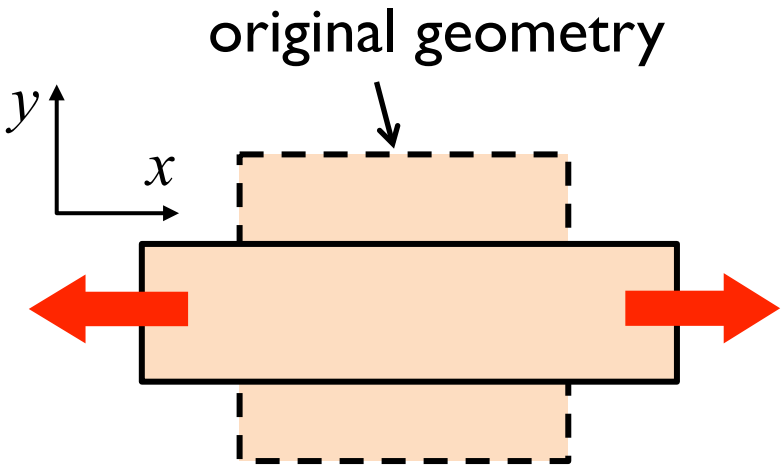
- Mechanical bending can tune conductivity in 2H MX_2.
- Experimental validation underway

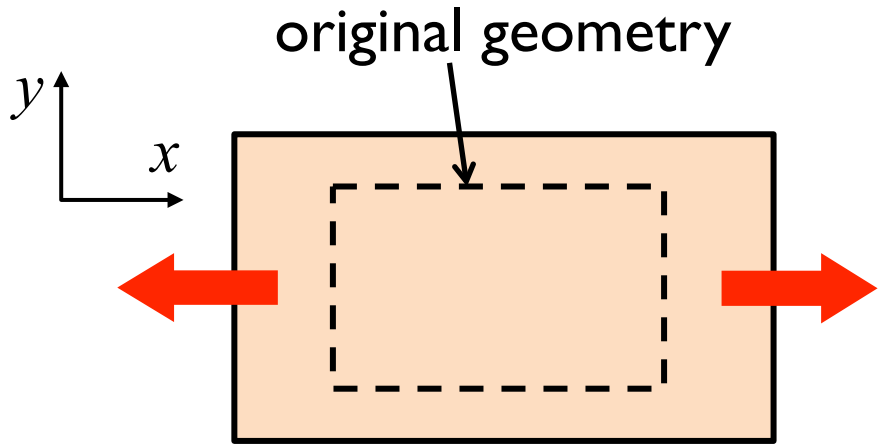
1T
octahedral



- 1T-MX_2 have unusual mechanical response.

Auxetics: Materials with a Negative Poisson's Ratio





Poisson's Ratio

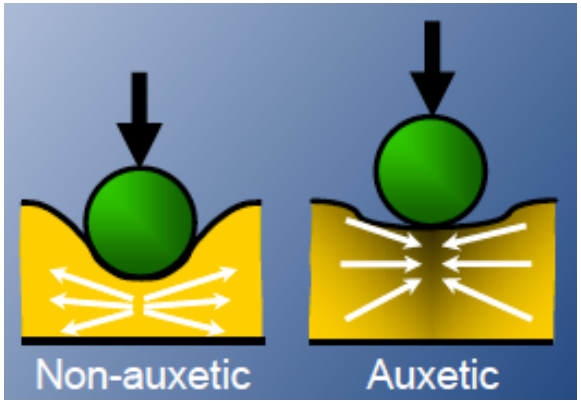
$$\nu_{yx} = -\frac{\varepsilon_y}{\varepsilon_x} > 0$$

- Non-auxetic

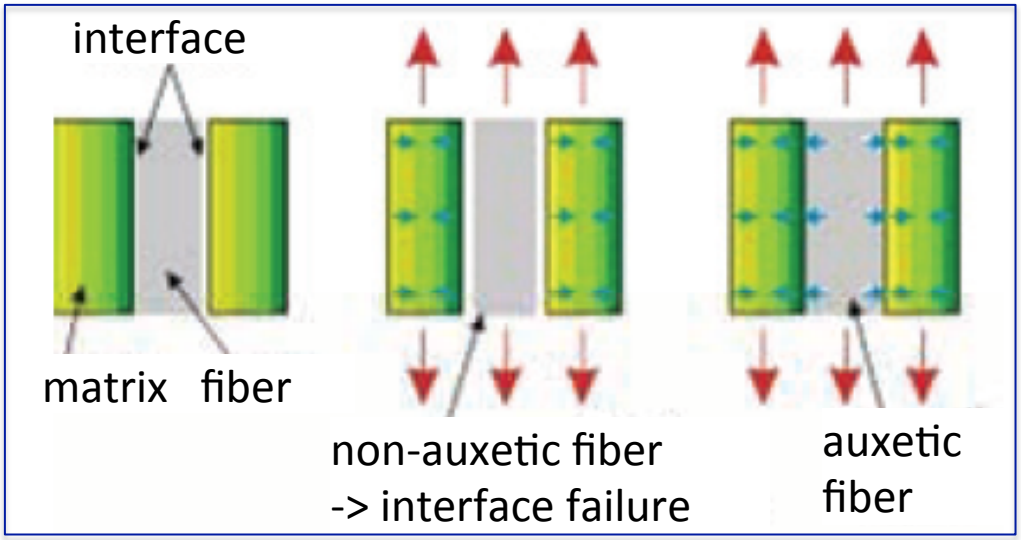
$$\nu_{yx} = -\frac{\varepsilon_y}{\varepsilon_x} < 0$$

- Auxetic
- counter-intuitive
- Unusual

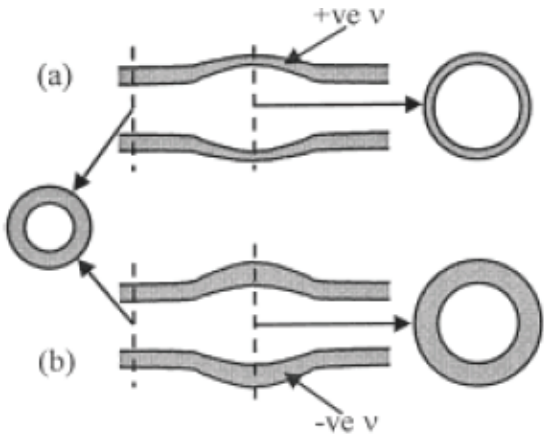
Potential Applications



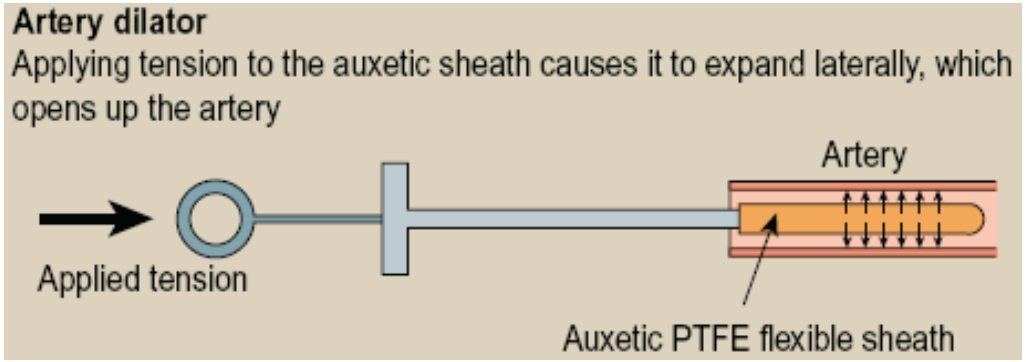
Bulletproof Vest & Armor Enhancement



Auxetic Fiber Reinforced Composites

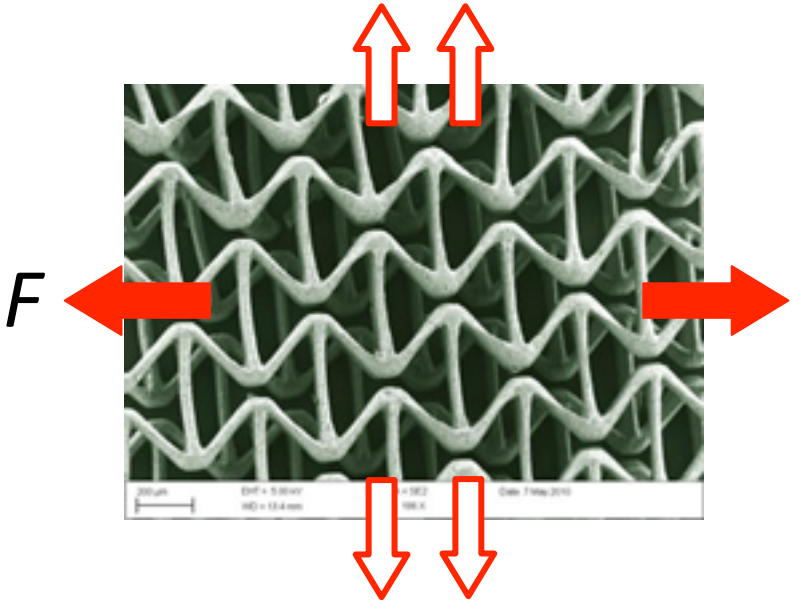


Artificial Blood Vessels

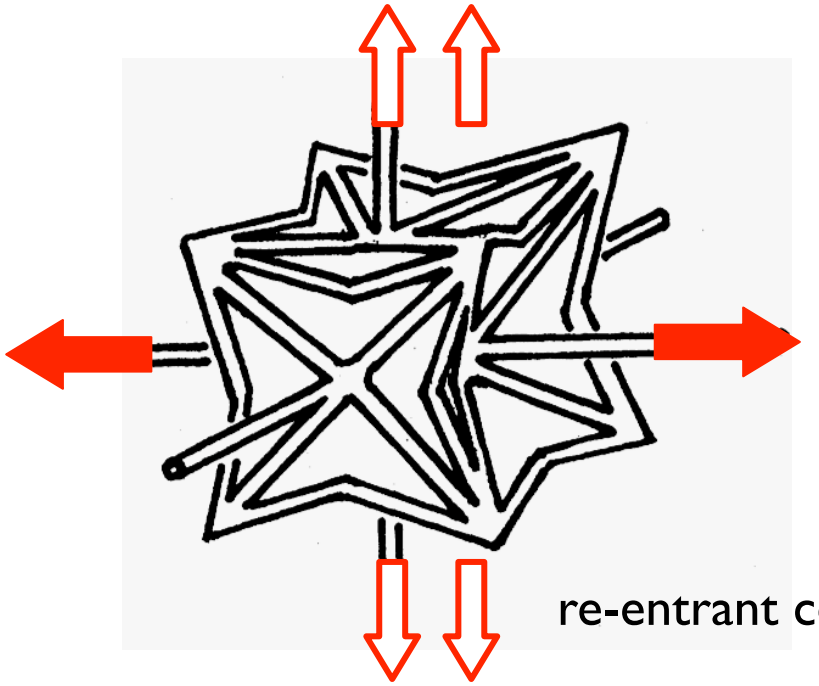


Artery Dilator

Common Structural Mechanisms



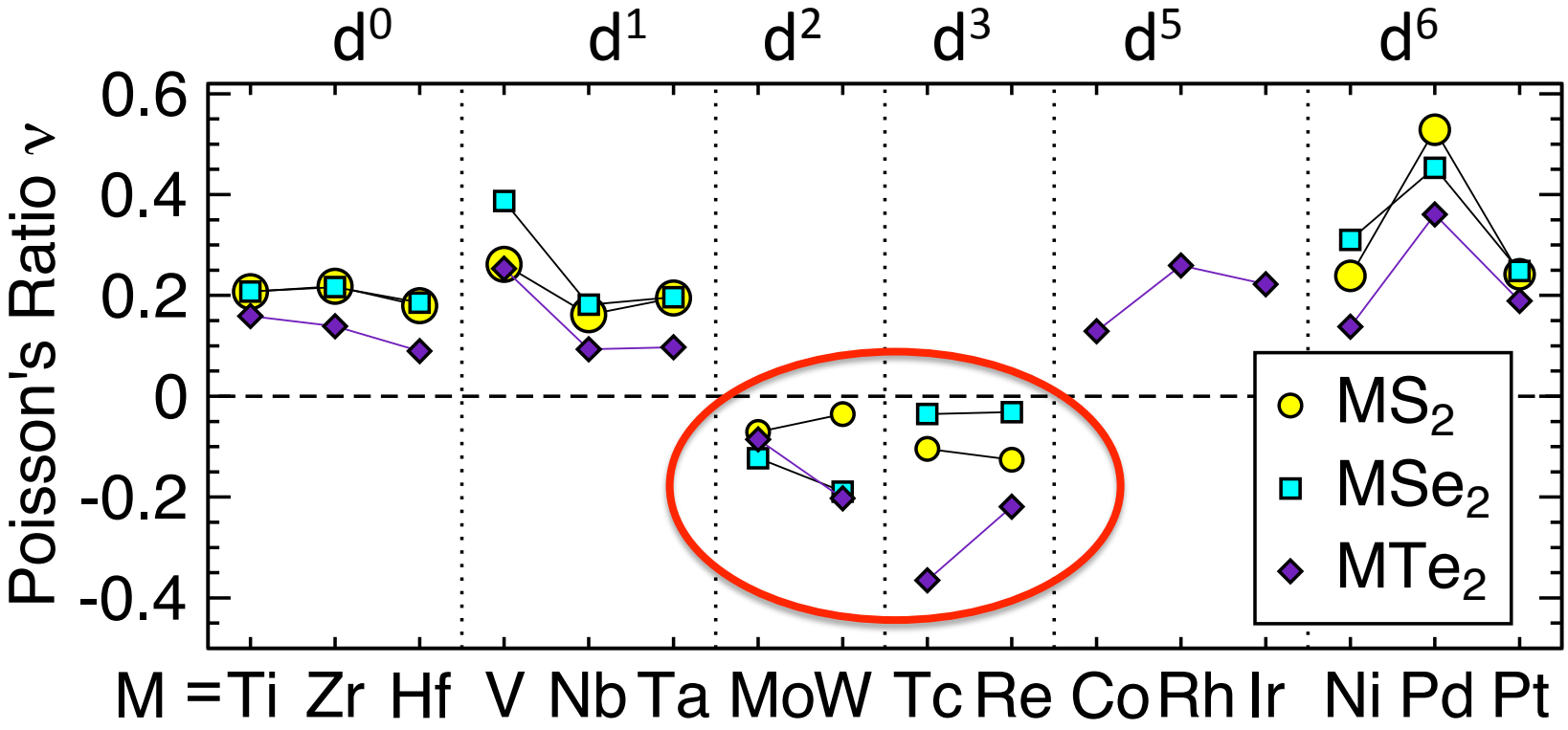
Polymer constructs
Adv. Funct. Mater, 21, 2712(2011)



Lakers, Science 235, 1038(1987)

- NPR is often considered as a purely geometric property.

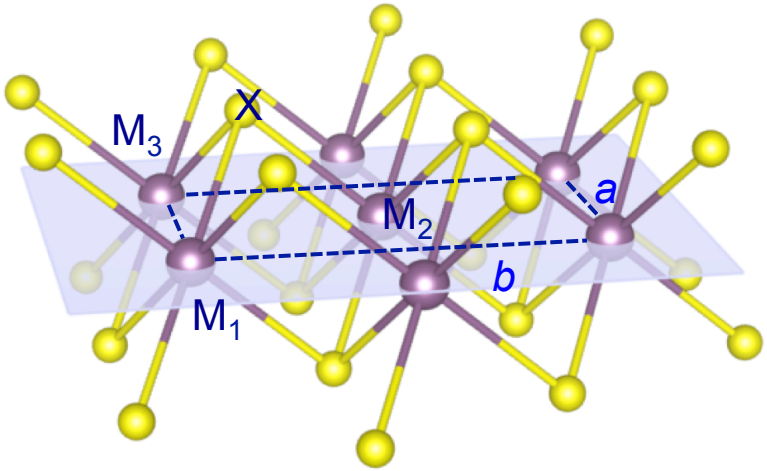
This work finds a new type of auxetic materials: 1T-MX_2



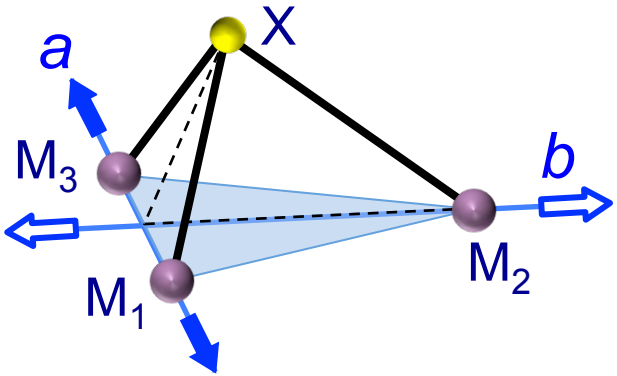
- Only d^2 and d^3 MX_2 compounds exhibit an intrinsic in-plane NPR.
- NPR is not a purely geometric property.

Yu, Yan & Ruzsinszky, *Nat. Communs.* 8, 15224 (2017).

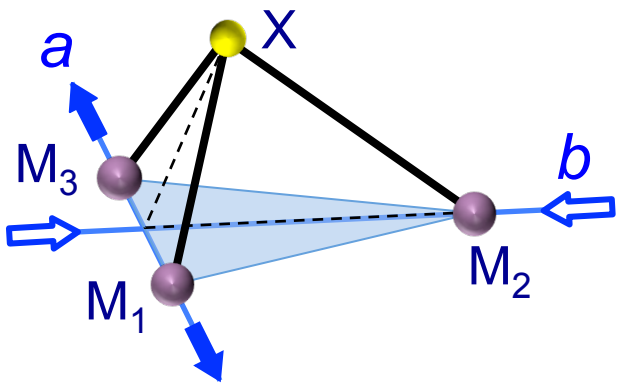
Structural Deformation Mechanism



Basic Building Unit :
X-$M_1M_2M_3$ triangular pyramid



auxetic

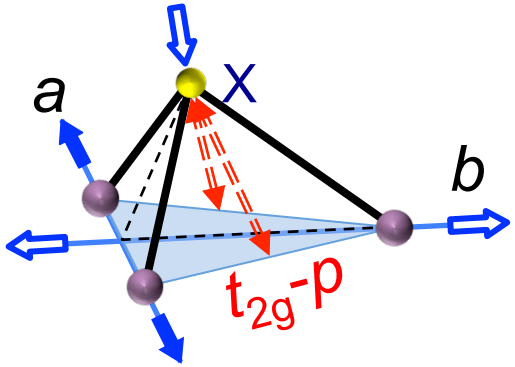


non-auxetic

Yu, Yan & Ruzsinszky, *Nat. Communs.* 8, 15224 (2017).

Electronic Origin: t_{2g}- p Interaction

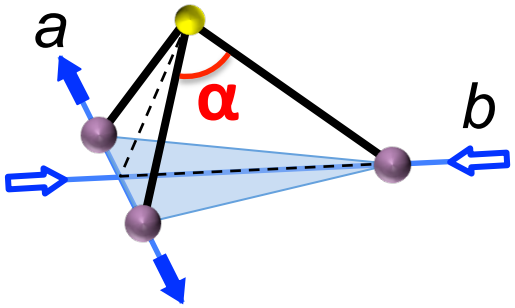
d^2-d^3 auxetic



- Strong t_{2g}-p orbital interaction attracts X atom toward the basal plane.

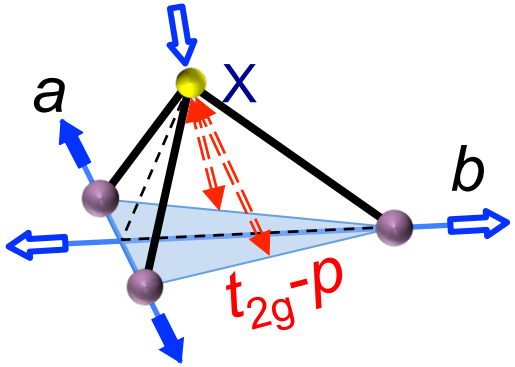
Electronic Origin: t_{2g}- p Interaction

d^0-d^1
non-auxetic



- Weak or marginal t_{2g}-p orbital interaction

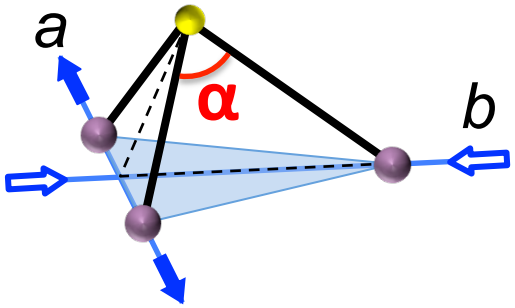
d^2-d^3
auxetic



- Strong t_{2g}-p orbital interaction attracts X atom toward the basal plane.

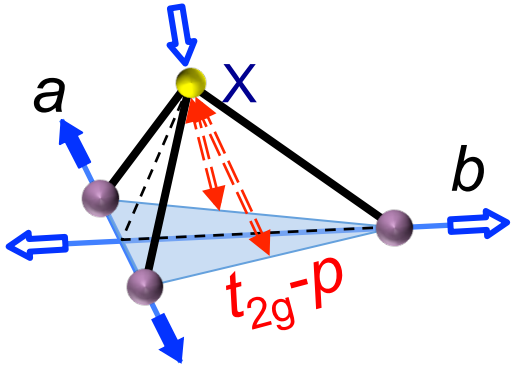
Electronic Origin: t_{2g}- p Interaction

d^0-d^1
non-auxetic



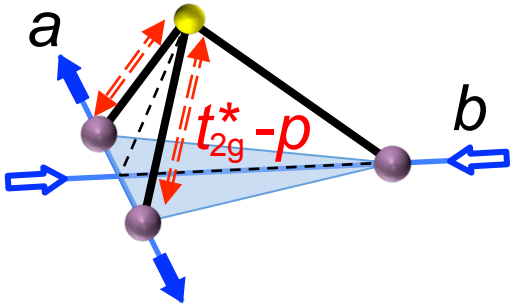
- Weak or marginal t_{2g}-p orbital interaction

d^2-d^3
auxetic



- Strong t_{2g}-p orbital interaction attracts X atom toward the basal phane.

d^5-d^6
non-auxetic



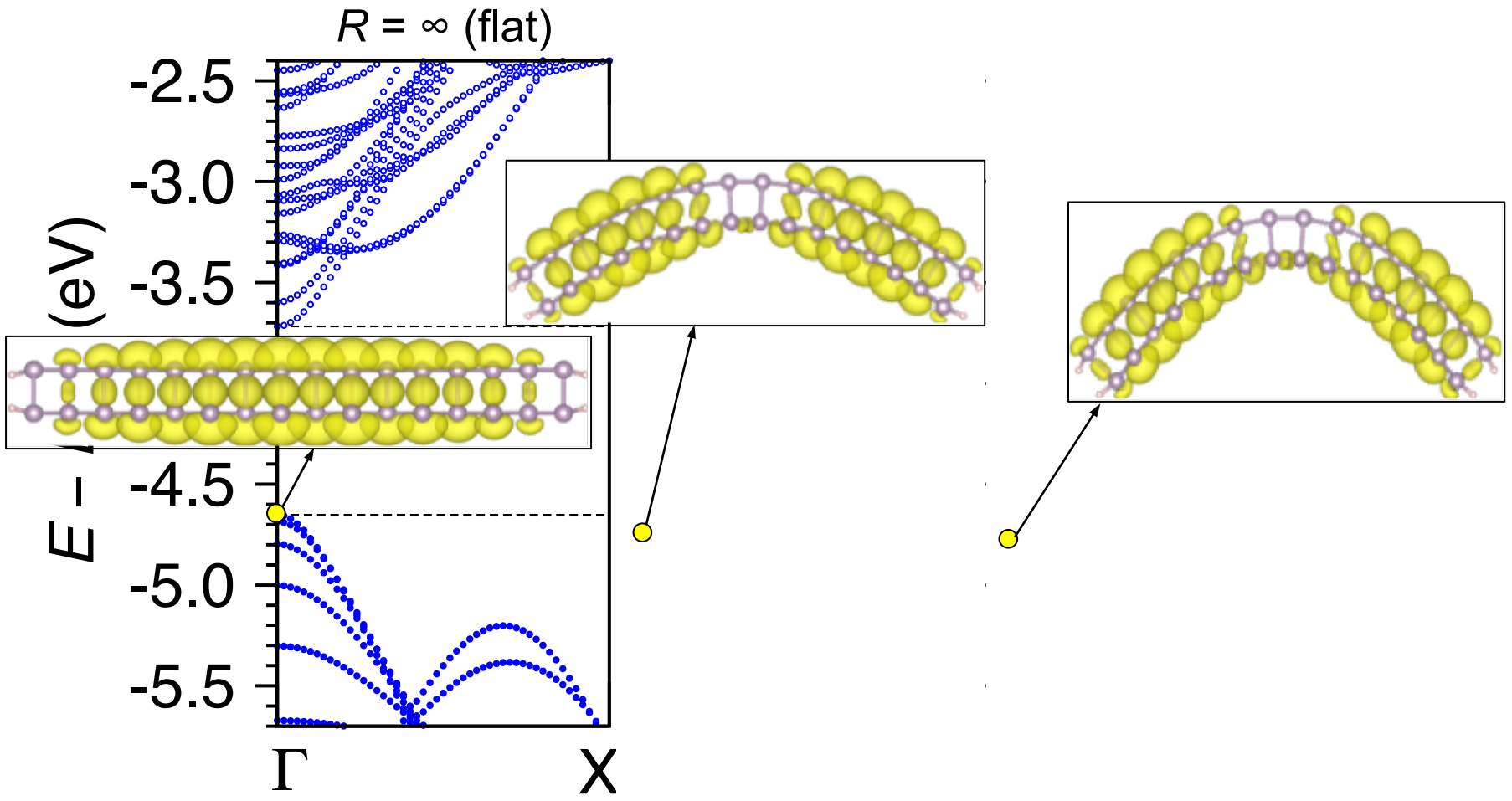
- Strong t_{2g}^*-p orbital interaction lies along the bond direction.

Conclusions

- Mechanical bending can be use to tune change charge localization (hence conductivity) in MoS_2 and phosphorene nanoribbons.

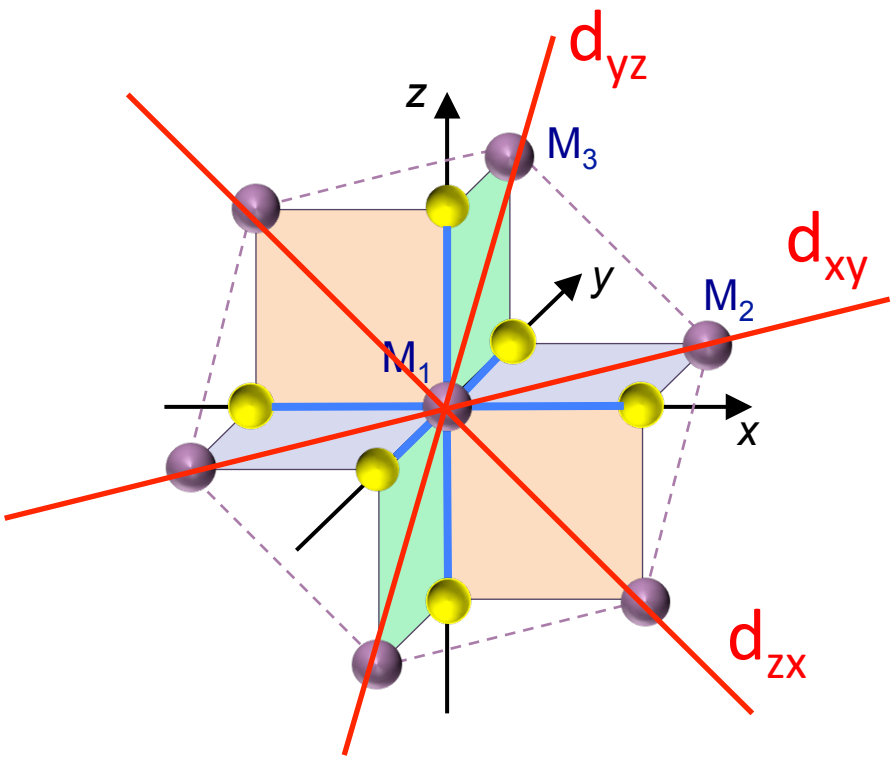
- d^2-d^3 1T-MX_2: a new type of auxetic 2D materials

Bending Localizes Hole Carriers in Phosphorene

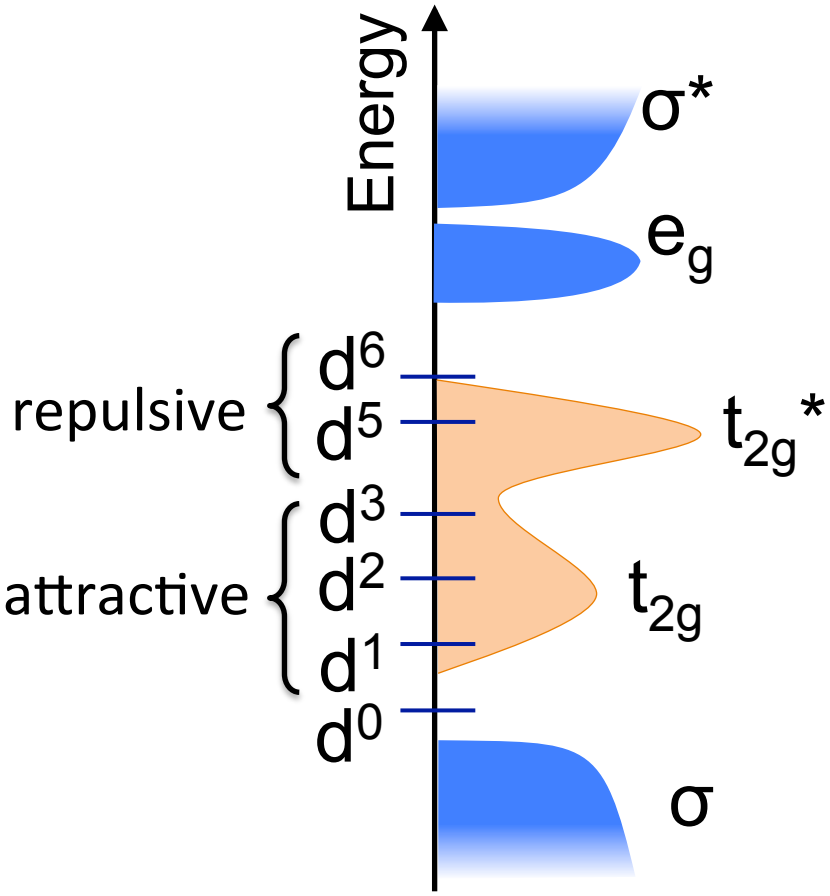


L. Yu, A. Ruzsinszky, J. Perdew, Nano Letters, 16, 2444(2016)

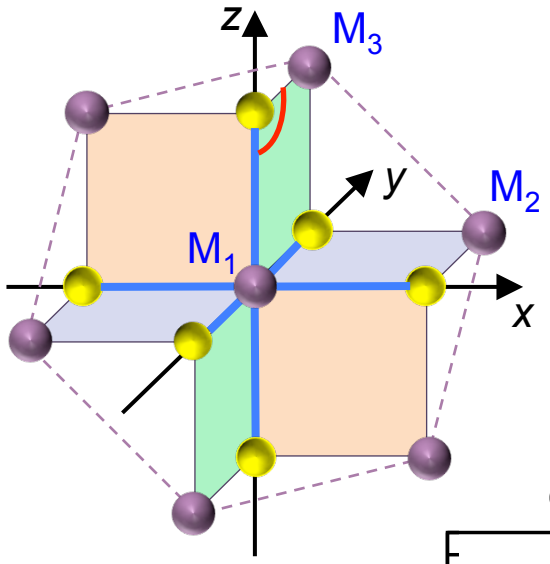
Intermetal t_{2g}-orbital Interaction



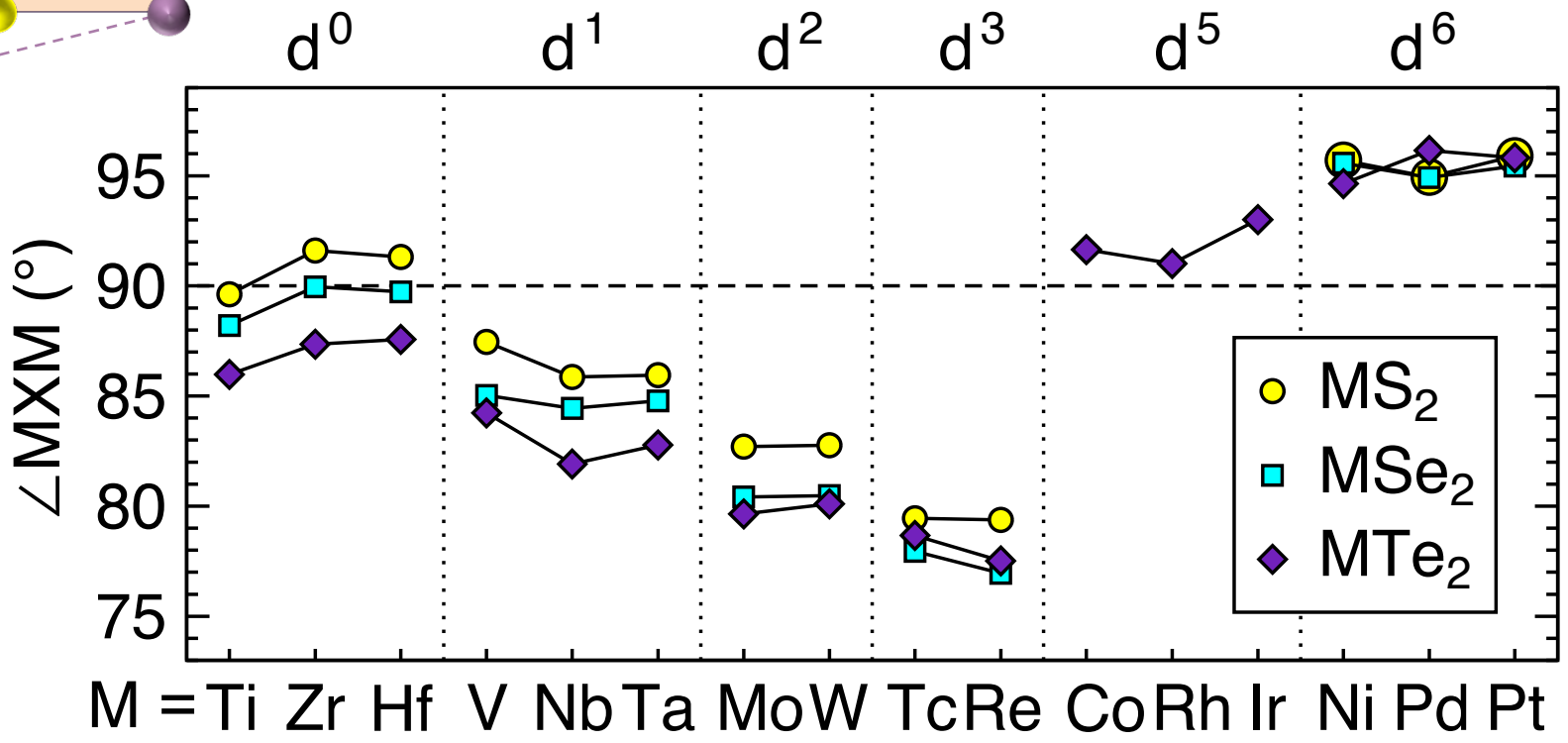
$M: d^n s^2 \rightarrow M^{4+}: d^{n-2} s^0$



Evidence of Intermetal t_{2g} Coupling



- M-X-M bond angles depend on d-electron count



Intermetal t_{2g}- p(X) Interaction