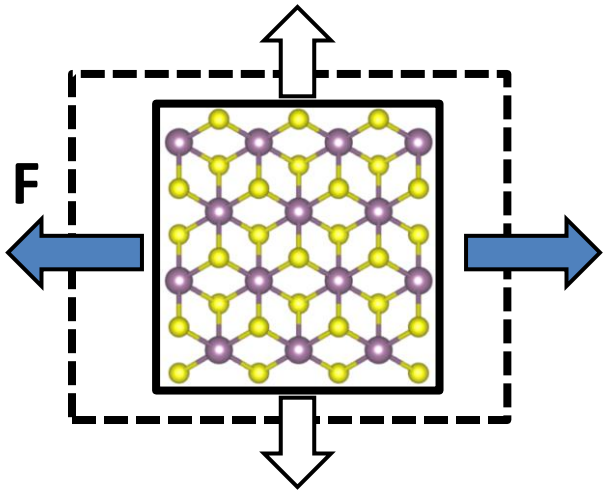
Unusual Negative Poisson's Ratio in 1T-Type Crystalline 2D Transition Metal Dichalcogenides



The figure schematically shows the unusual and counter-intuitive mechanical behavior of a material with negative Poisson's ratios. It expands laterally when stretched longitudinally. Materials with such behavior are also called as auxetics.

L. Yu, Q. Yan, and A. Ruzsinszky, *Nature Communications* 8, 15224 (2017)
doi:10.1038/ncomms15224

Work was performed at Temple University

Scientific Achievement

First-principles calculations predicts a new class of auxetic single-layer two-dimensional materials, namely, the 1T-type monolayer crystals of groups 6–7 transition-metal dichalcogenides, MX_2 (M=Mo, W, Tc, Re; X=S, Se, Te).

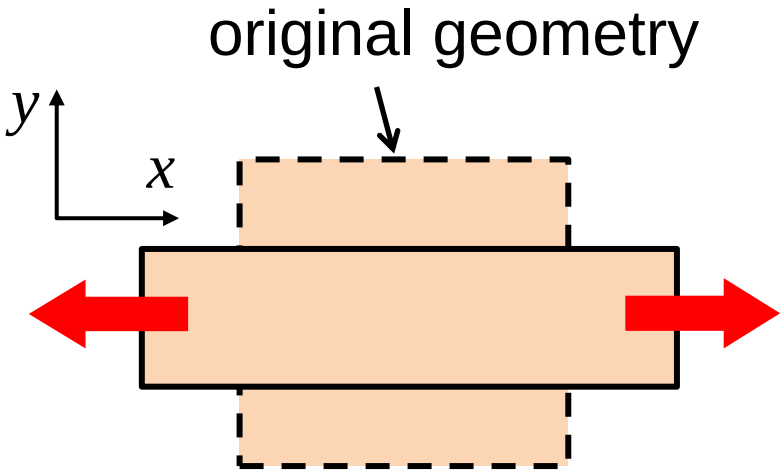
Significance and Impact

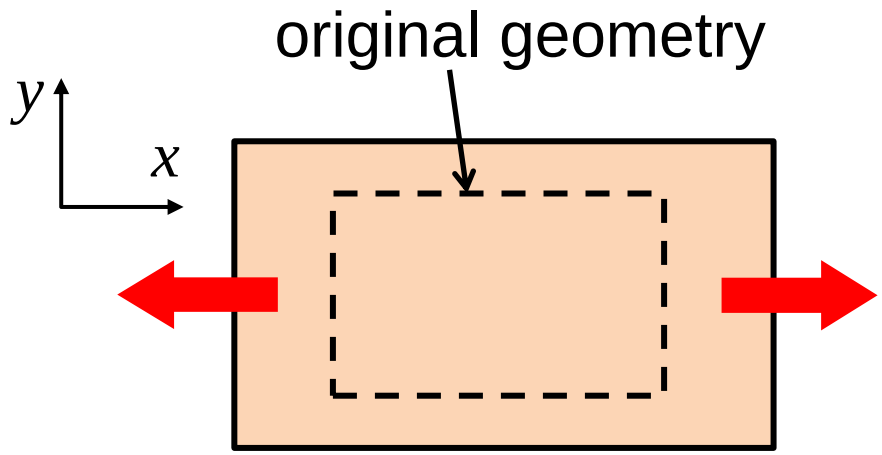
The auxetic behaviour in combination with other remarkable properties of monolayer two-dimensional materials could lead to novel multi-functionalities (e.g., auxetic electronics).

Research Details

- 12 of 42 possible 1T-MX_2 are predicted to be auxetic. Others (albeit having the same crystal structure) are non-auxetic.
- The in-plane stiffness of auxetic 1T-MX2 materials is predicted to be order of 10^2 GPa, at least three orders of magnitude higher than man-made auxetic materials.
- The auxetics originates from the strong coupling between the chalcogen p orbitals and the intermetal t_{2g}-bonding orbitals within the basic triangular pyramid structure unit.

Auxetics: Materials with a Negative Poisson's Ratio





Poisson's Ratio

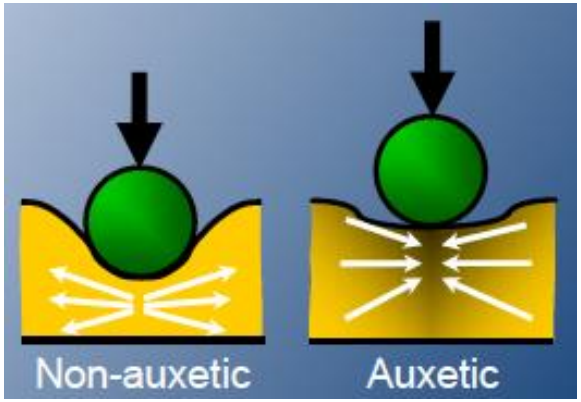
$$n_{yx} = -\frac{e_y}{e_x} > 0$$

- Non-auxetic

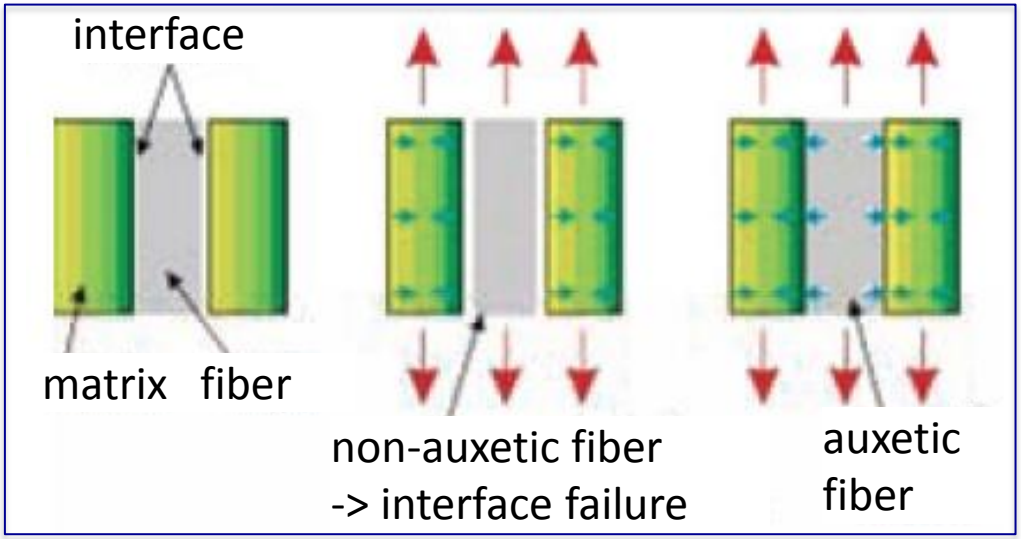
$$n_{yx} = -\frac{e_y}{e_x} < 0$$

- Auxetic
- counter-intuitive
- Unusual

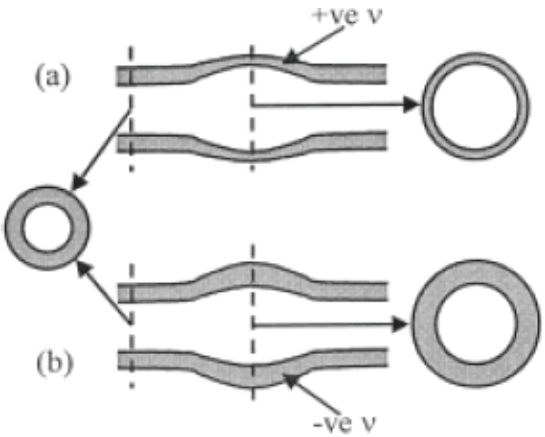
Potential Applications



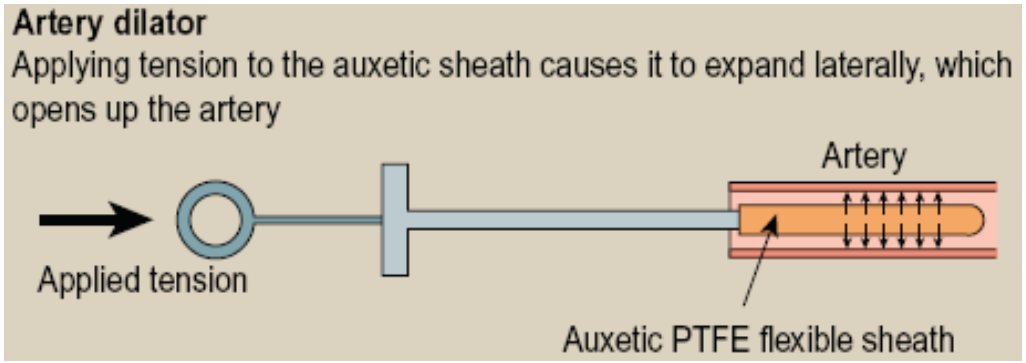
Bulletproof Vest & Armor Enhancement



Auxetic Fiber Reinforced Composites

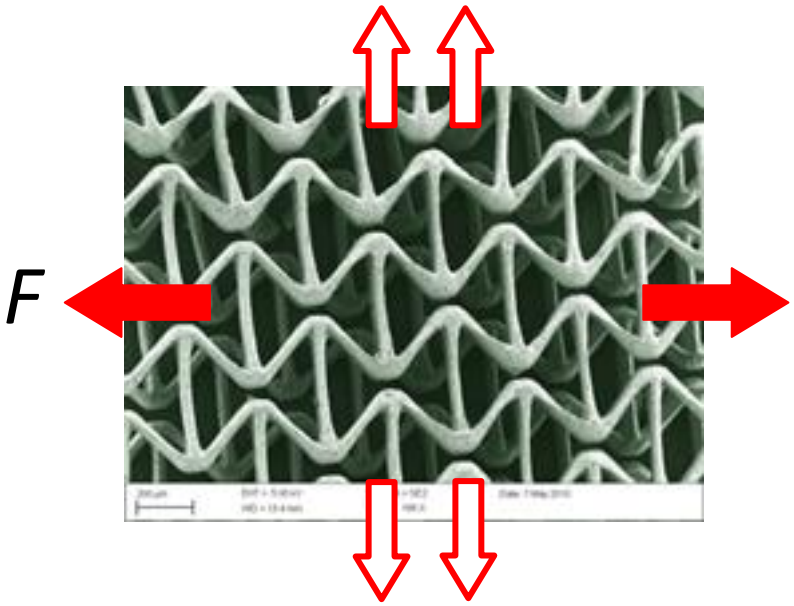


Artificial Blood Vessels

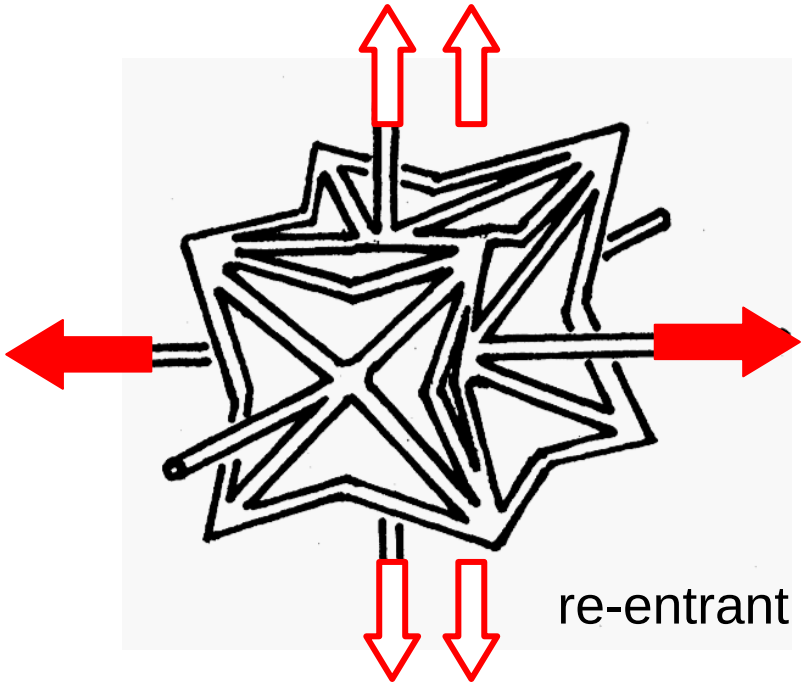


Artery Dilator

Common Structural Mechanisms



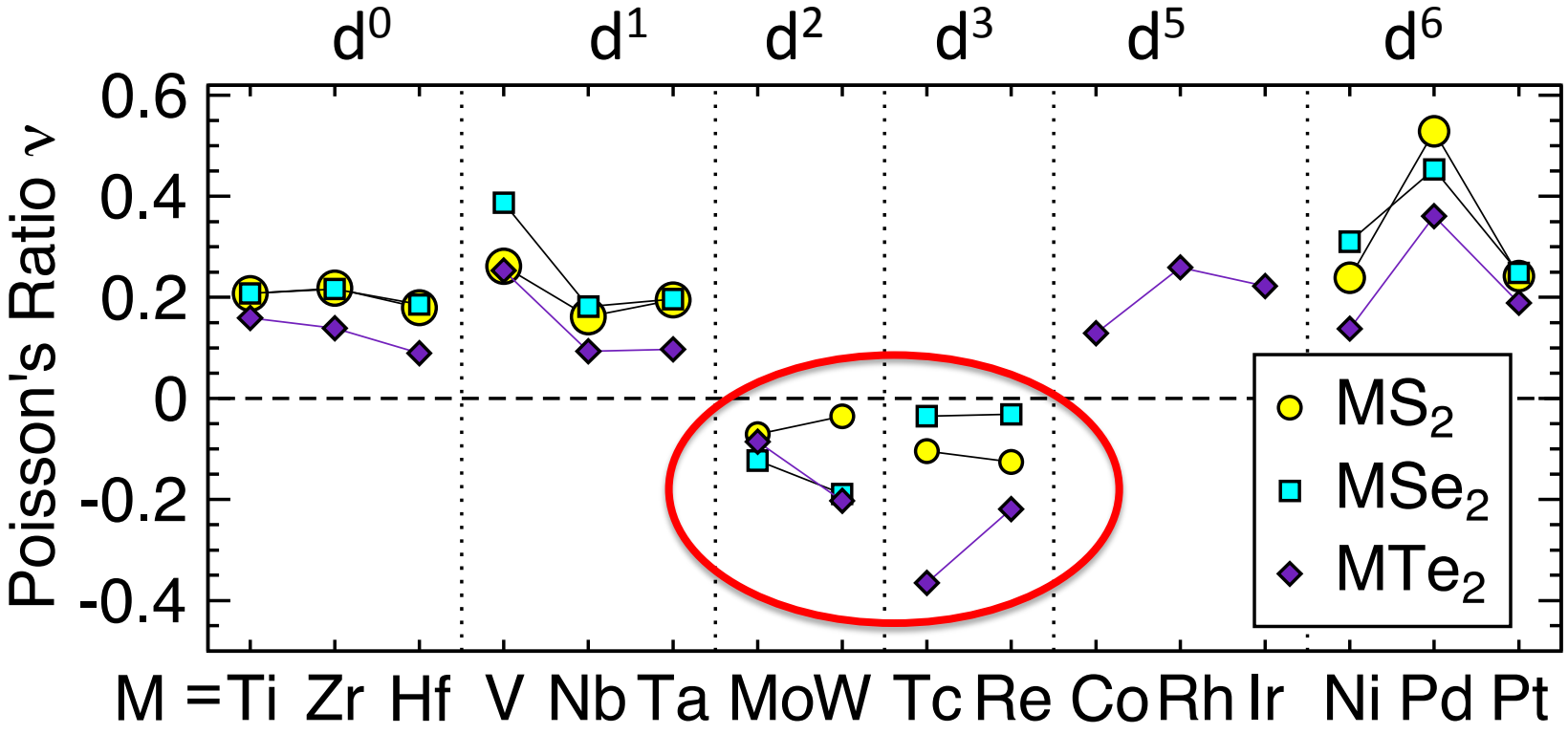
Polymer constructs
Adv. Funct. Mater, 21, 2712(2011)



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.

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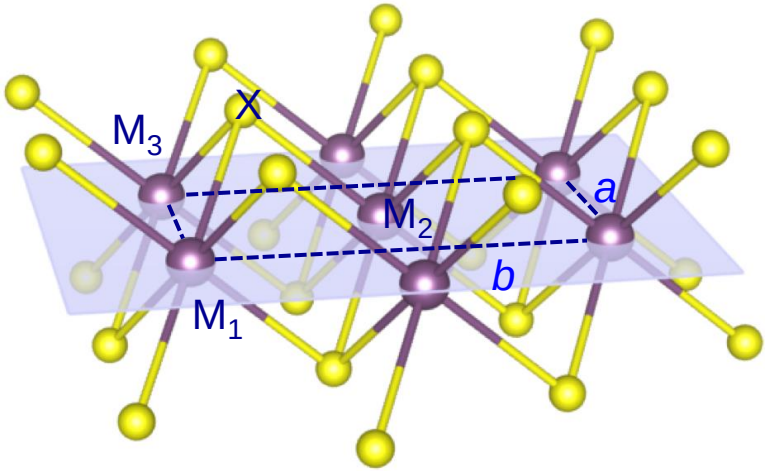
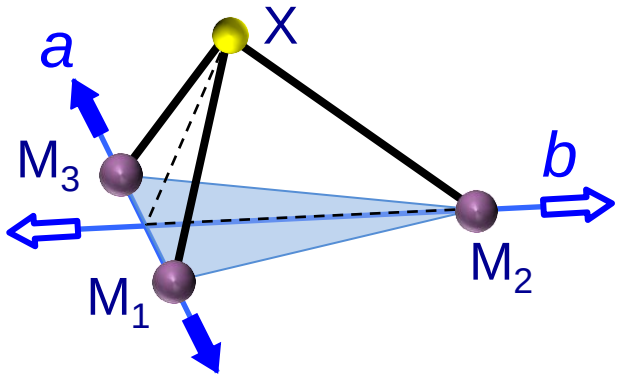
Yu, Yan & Ruzsinszky, *Nat. Communs.* 8, 15224 (2017)

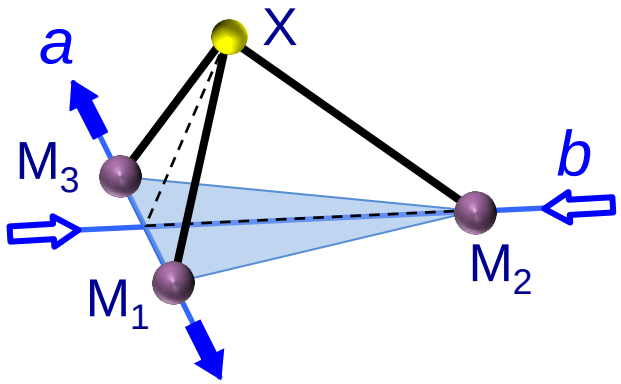
Structural Deformation Mechanism





auxetic

Basic Building Unit : X-$M_1M_2M_3$ triangular pyramid

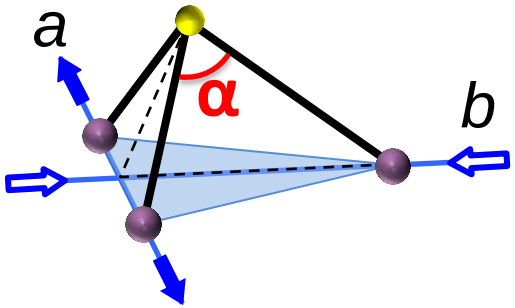


non-auxetic

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

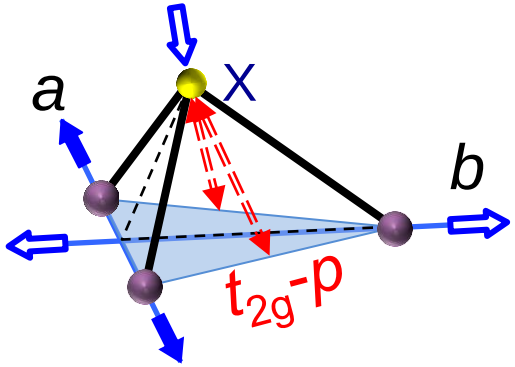
Electronic Origin: t_{2g}- p Interaction

d^0-d^1 non-auxetic



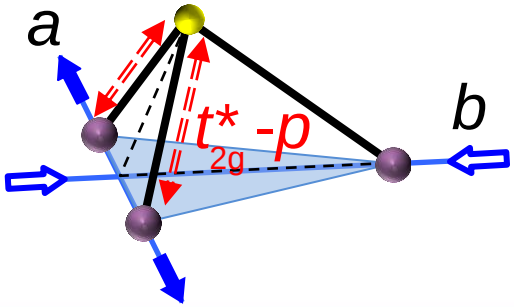
- Weak or marginal t_{2g}-p orbital interaction

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.

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