Phase Change and Piezoelectric Properties of Two-Dimensional Materials

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Many single layer materials exhibit emergent piezoelectricity, e.g. MoS$_2$

Some single layer materials (e.g. MoTe$_2$) exhibit structural metal-insulator phase transitions under tensile strains.
  - Duerloo, Li, Reed, *Nat. Comm.* 5, 4214 (2014);
PIEZOELECTRIC MATERIAL APPLICATIONS

Stress Sensors

Acoustic transducers for signal processing

Scanning Tunneling Microscope (STM)

Injet Printing
Piezoelectric materials must exhibit:

1. An electronic bandgap
2. A lack of centrosymmetry

Inversion symmetry of a crystal => $d_{ijk} = (-1)^3 d_{ijk} = -d_{ijk}$

So $d_{ijk}=0$ for crystals with inversion symmetry!
GRAPHENE IS NOT PIEZOELECTRIC

- Inversion symmetry => non-piezoelectric
- Semi-metallic character => non-piezoelectric
Transition Metal Dichalcogenides: MoS$_2$, MoSe$_2$, MoTe$_2$, WS$_2$, WSe$_2$

Trigonal prismatic structure:

- Semiconducting ($E_{\text{gap}} \sim 1$-2 eV)
- Not centrosymmetric
- 3m point group leads to non-zero $d_{11}$ and $e_{11}$ coefficients
Our HPC-enabled approach enables identification of promising materials. We discover that a variety of TMDS have significant piezoelectric effects.

Piezo-coefficients of trigonal prismatic TMD structures are comparable to bulk wurtzite structures.


Reported $e_{11}$ within 20% of predicted.


Piezoelectricity in C$_3$N$_4$ few layers:
We find that TMDC monolayers are piezoelectric while their bulk host crystals exhibit an inversion center and are therefore not piezoelectric!

We predict bilayer BN exhibits an electromechanical curvature effect.

TMD MONOLAYERS CAN EXIST IN MULTIPLE CRYSTAL STRUCTURES

A FRONTIER: SURFACE CHEMISTRY

BEYOND PLANE-WAVE DFT

TMD MONOLAYERS CAN EXIST IN
MULTIPLE CRYSTAL STRUCTURES

2H

1T

1T'

Semiconducting
(1-2 eV)

Metallic

Semi-metallic

distortion
Two phases have been observed in chemically exfoliated MoS$_2$ and WS$_2$.

Eda et al, ACS Nano 6, 7311 (2012);
CAN TENSILE STRAIN CAUSE A STRUCTURAL PHASE TRANSITION?
Our DFT/PBE calculations of TMD monolayer phase boundaries in strain.

Energy calculations on a 5x5 grid in (a,b) lattice constants. Lagrange interpolation for phase boundaries.

Tensile strain of 6% along b axis crosses phase boundary in MoTe$_2$.

Hybrid exchange (HSE06) moves phase boundary closer to ambient conditions.

- Incorporation of entropic effects (F=E-TS) accomplished using quasiharmonic approximation with computed phonon bands.

HSE06 with room T vibrations predict phase boundary within 3% tensile strain in MoTe$_2$. 

\[ F(a, b) \approx U_{\text{crystal}}(a, b) + \sum_i \left[ \frac{1}{2} \hbar \omega_i(a, b) + k_B T \ln \left( 1 - e^{-\hbar \omega_i(a, b)/k_B T} \right) \right] \]
New materials are needed to mitigate escalating power requirements for electronic devices.

Metal-oxides: VO$_2$

Chalcogenide alloys: Ge$_2$Sb$_2$Te$_5$ (GST)

Suitable phase change materials are rare animals. We discover a promising new material.

Application spaces:
- Information and energy storage
- Low power electronics
- Infrared technologies
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CONCLUSIONS

- Many single layer materials exhibit emergent piezoelectricity, e.g. MoS$_2$

- Some single layer materials (e.g. MoTe$_2$) exhibit structural metal-insulator phase transitions under tensile strains.