CTU
CZECH TECHNICAL UNIVERSITY IN PRAGUE

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MINISTRY OF EDUCATION, YOUTH AND SPORTS

Predicting Tribological Properties of Low-Dimensional Materials

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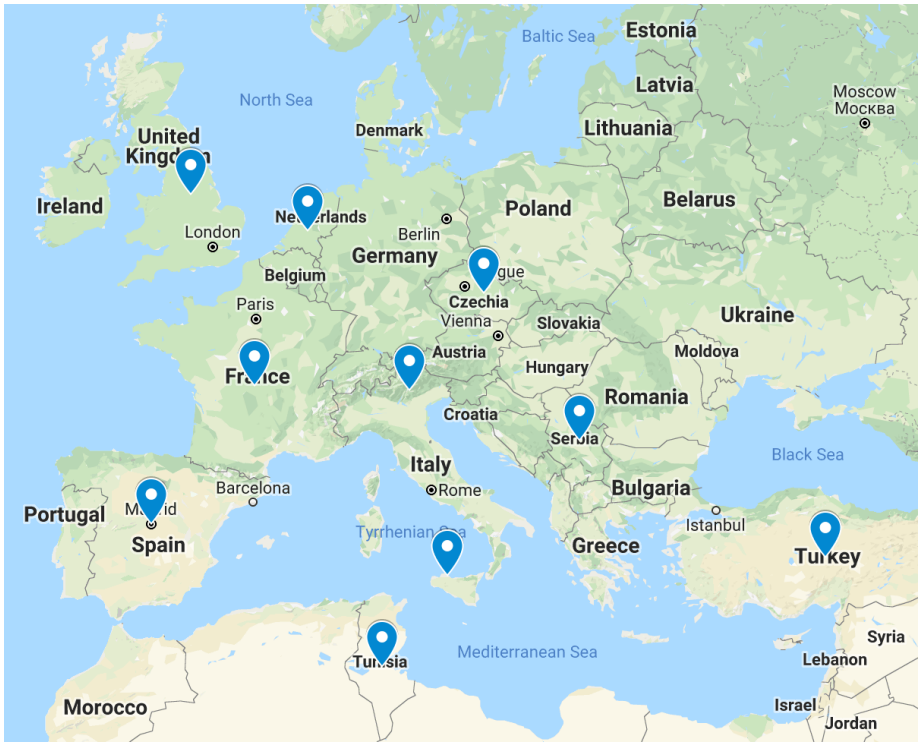
Advanced Materials Group



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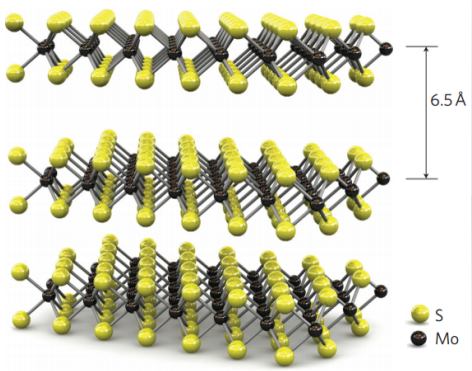
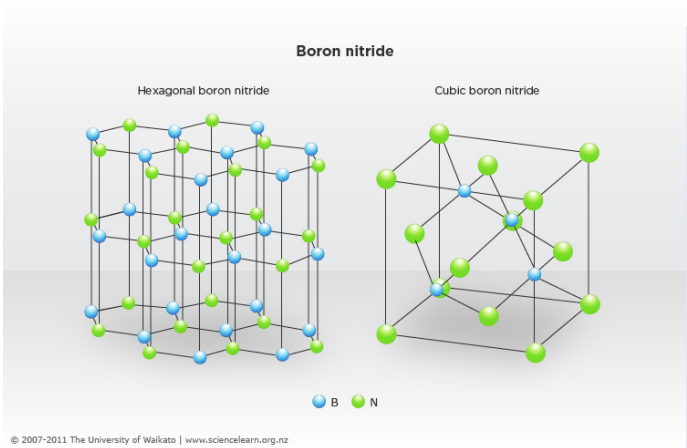
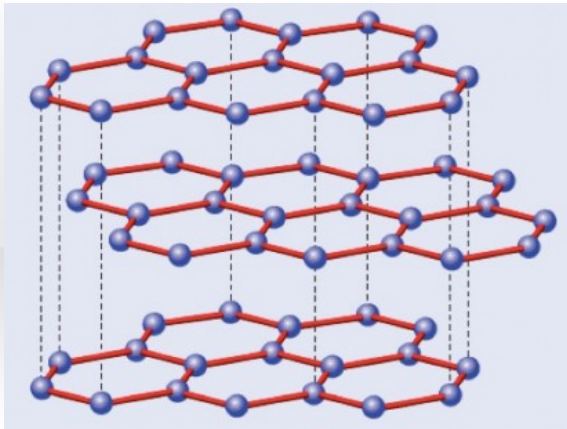
Advanced Materials Group

- Self-adaptive low-friction coatings [WSC; WSeC; MoSC; MoSeC]
- High temperature tribology
- Biocompatible coatings
- Interface design of crystalline materials with improved radiation damage resistance
- **Modelling & Simulations** *e.g.* TMD; h-BN; ZnO; Graphene







Studying materials *in silico*

- Methods generally fall into two distinct categories:
- **Quantum:** uses quantum physics; suitable for smaller systems (10-100s of atoms) parameter-free (can do 'brand new' chemistry & physics); computationally intensive
- **Classical:** uses classical physics; suitable for larger systems ($10^2 - 10^6$ of atoms); computationally less intensive; no electronic properties; may be less accurate
- In Advanced Materials Group we combine both methods

Studying materials *in silico*

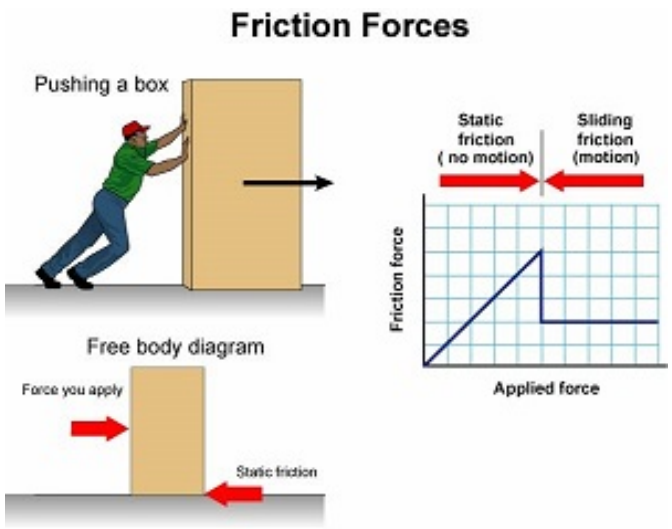
- Simulation packages: LAMMPS, VASP, ABINIT, SIESTA...
- High Performance Computing clusters (ca. 10^7 CPU hrs):
  Anselm/Salomon, IT4I, Ostrava, CZ
  Iridis, University of Southampton, UK
  Eagle, Poznań, Poland

Projects @ IT4Innovations

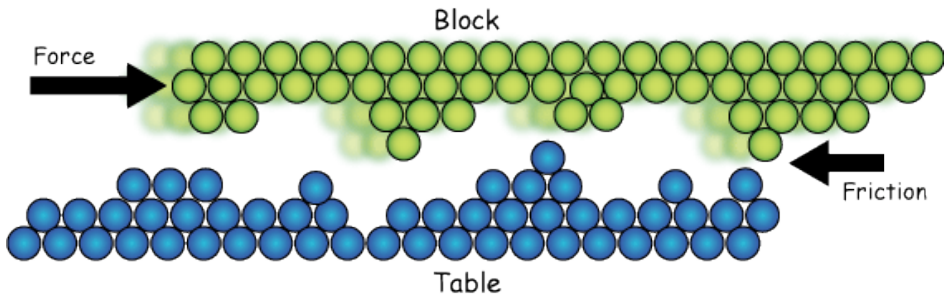
- CODFISH (2,5 M); ENDFISH (0,5 M)
- HOLDEM (2,23 M)
- OPTOSILICA (0,5 M)
- FATRADEX (2,5 M)
- NanoTribo (1,5 M)
- ATRIO (3,03 M)
- RATONMO (2,83 M)
- AFAM (2,706 M)

Background

- **Friction:** a force that resists sliding or rolling of one object over another; both a necessity and a disadvantage
- **Tribology:** from Greek $\tau\rho\iota\beta\omega$ ('I rub') + $\lambda o\gamma\iota\alpha$ ('study of'); the multidisciplinary (engineering, metallurgy, chemistry) study of interactions between sliding surfaces



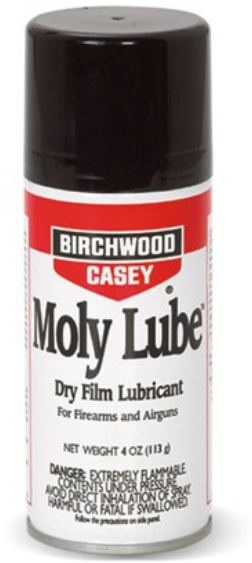
study.com

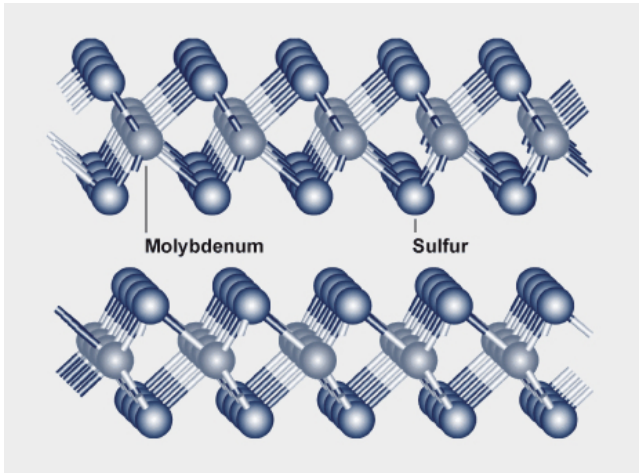


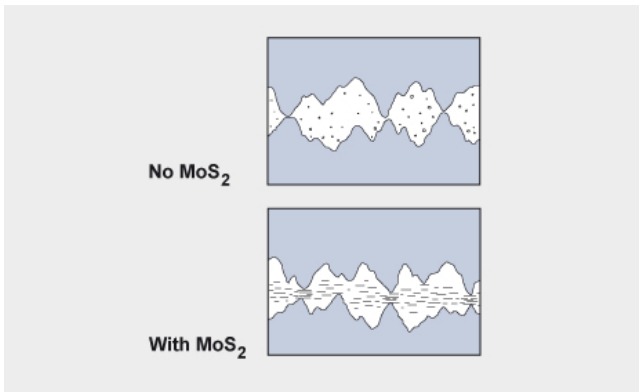
drcruzan.com

TMDs - structure & lubricating properties [AMG]

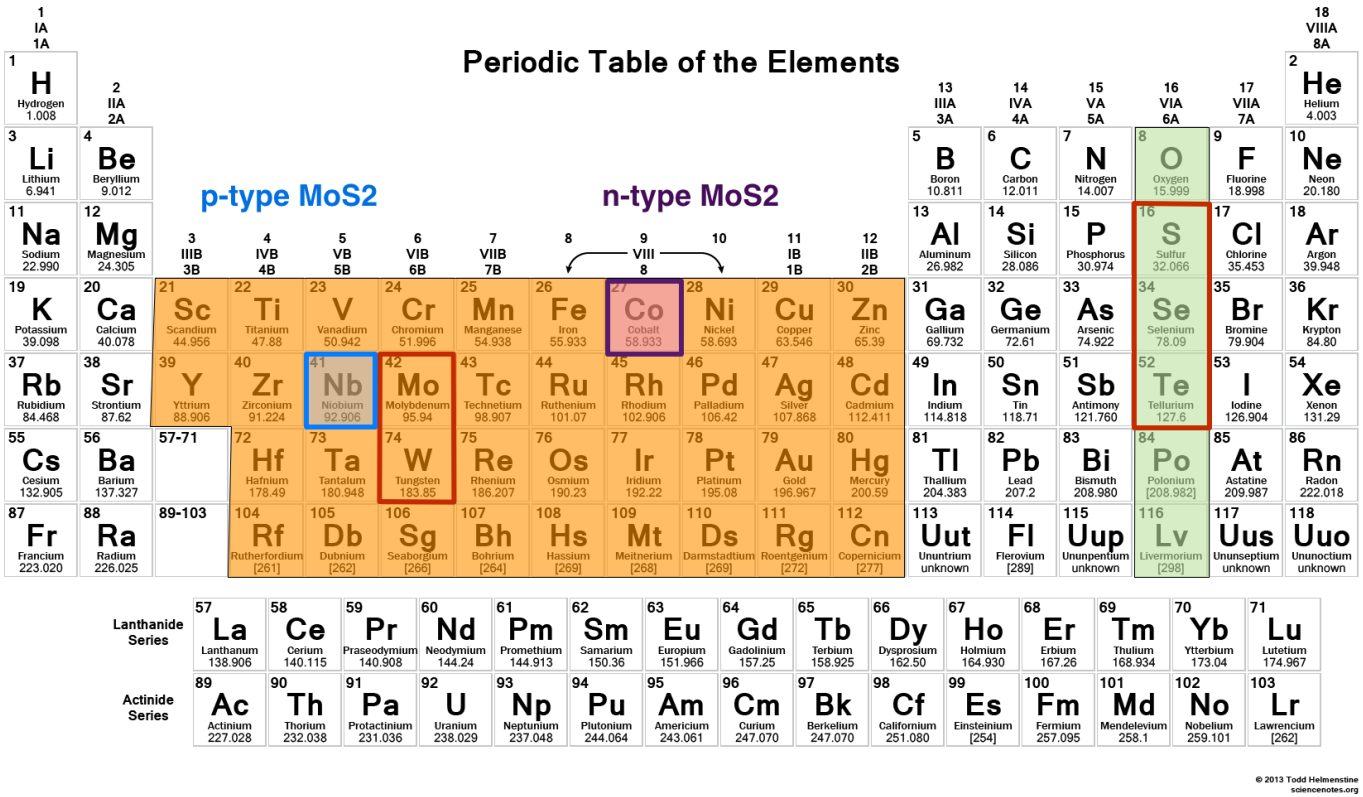
- MX_2 family of compounds, where M = Mo, W; X = S, Se, Te
- Molybdenum disulfide, MoS_2, best known example

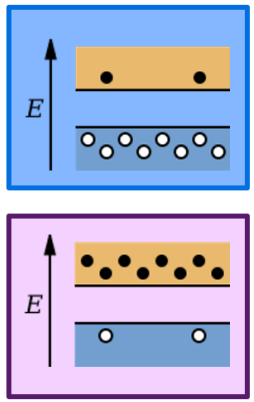






TMDs - structure & physicochemical properties

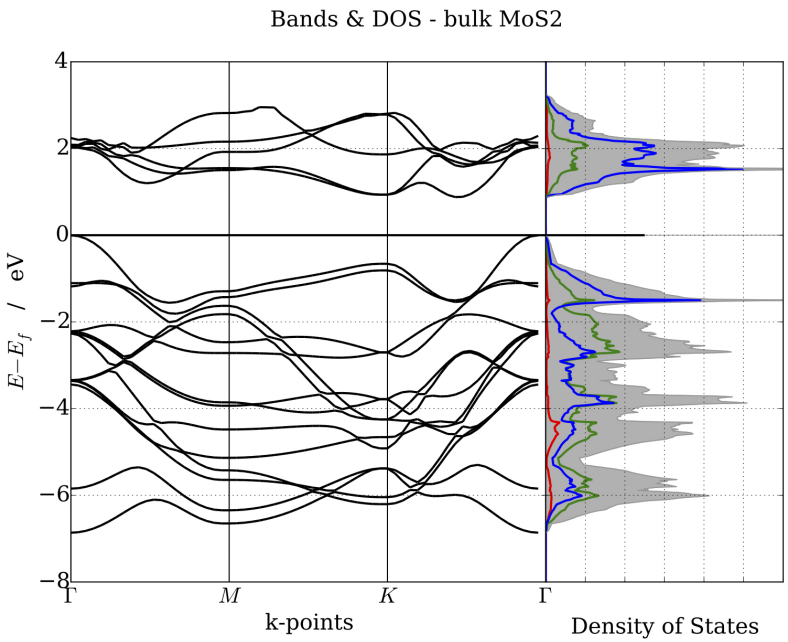


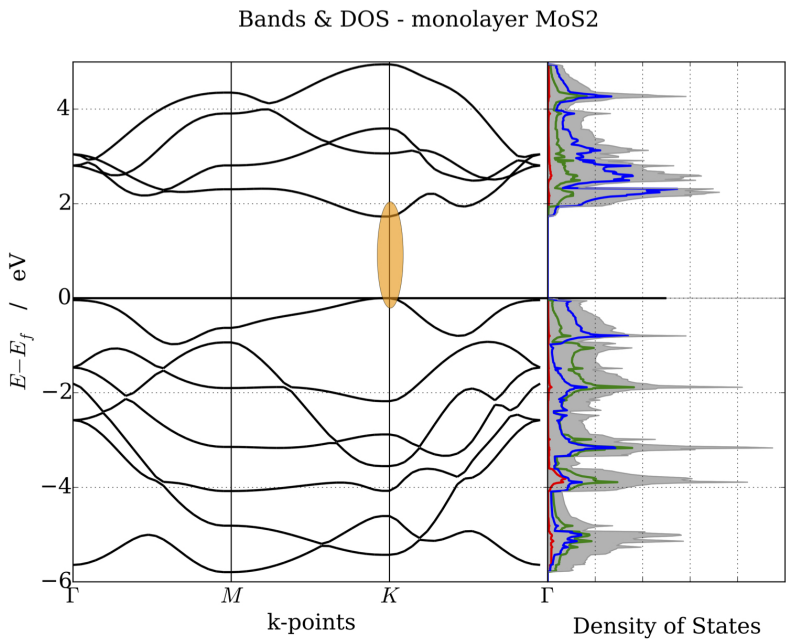


- We have a variety of stoichiometries available, each offering unique properties
- We can explore/improve their properties using both experiments and theory

Homogeneous TMDs

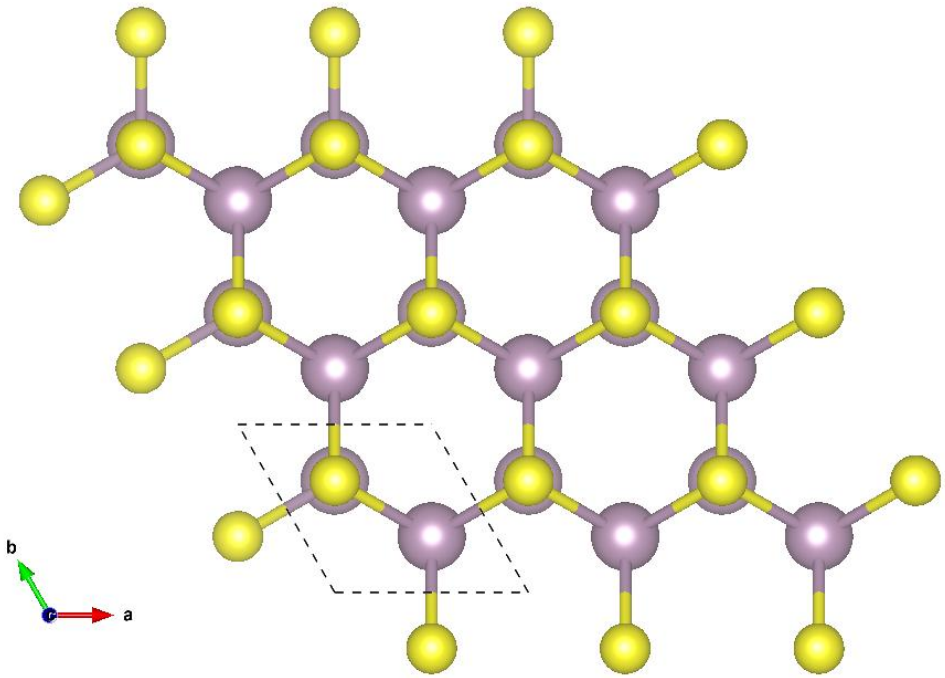
- Layer-dependent properties of TMDs have attracted much attention e.g. MoS_2 transition from indirect (1.3 eV) to direct bandgap (1.8 eV):

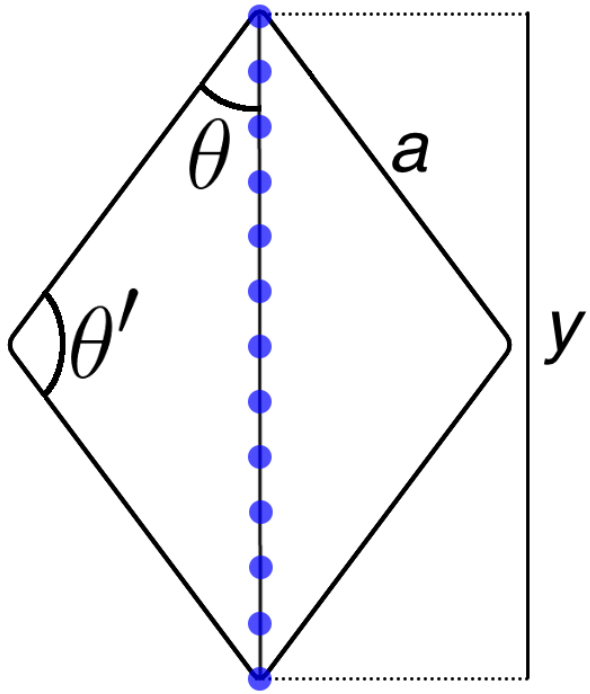




Nanoscale (DOI: 10.1039/c7nr00925a)

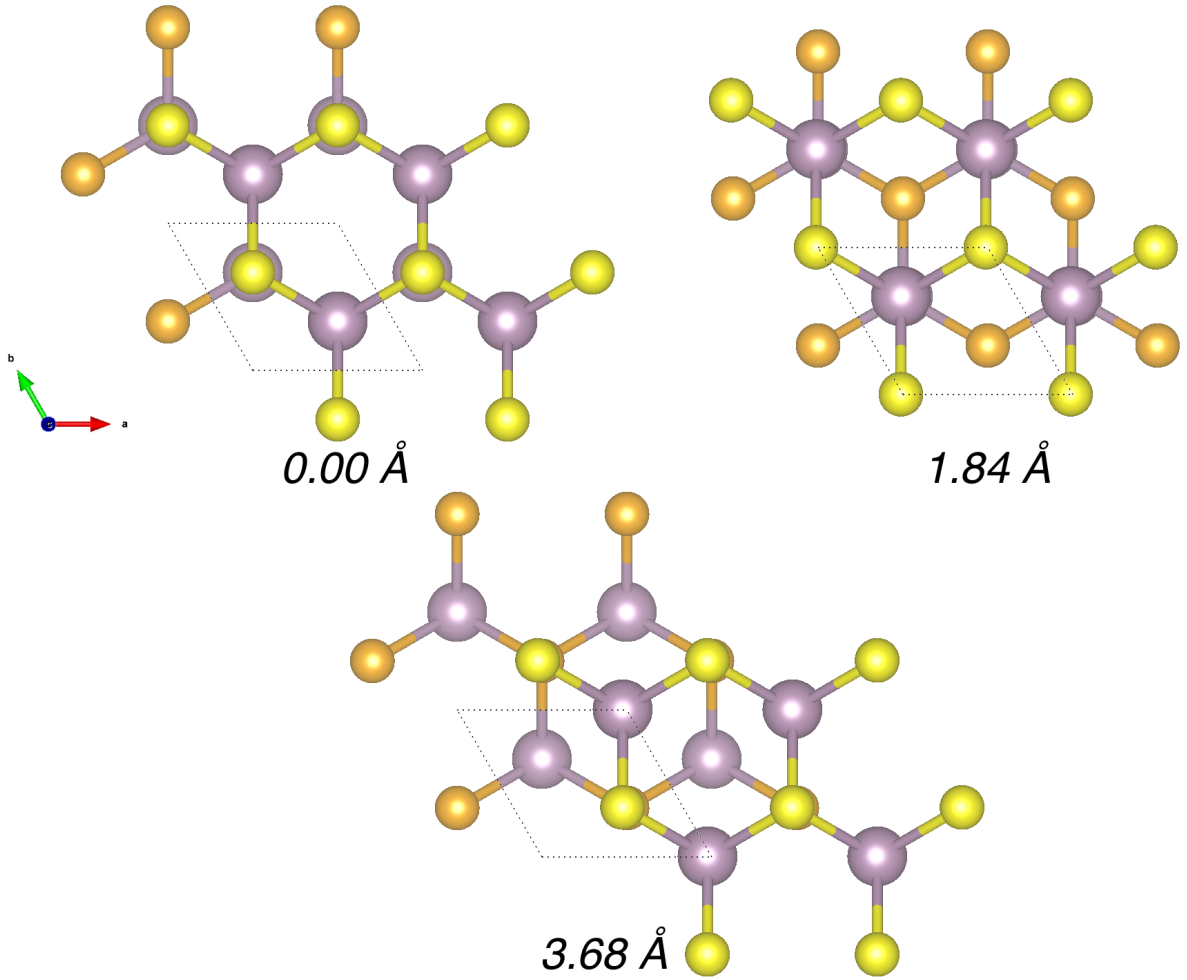
Recent work - DFT calculations to investigate sliding properties of TMDs





Nanoscale (DOI: 10.1039/c7nr00925a)

Most important geometric configurations for MX_2 bilayers:



Nanoscale (DOI: 10.1039/c7nr00925a)

Potential energy profiles for MoX_2 bilayers:

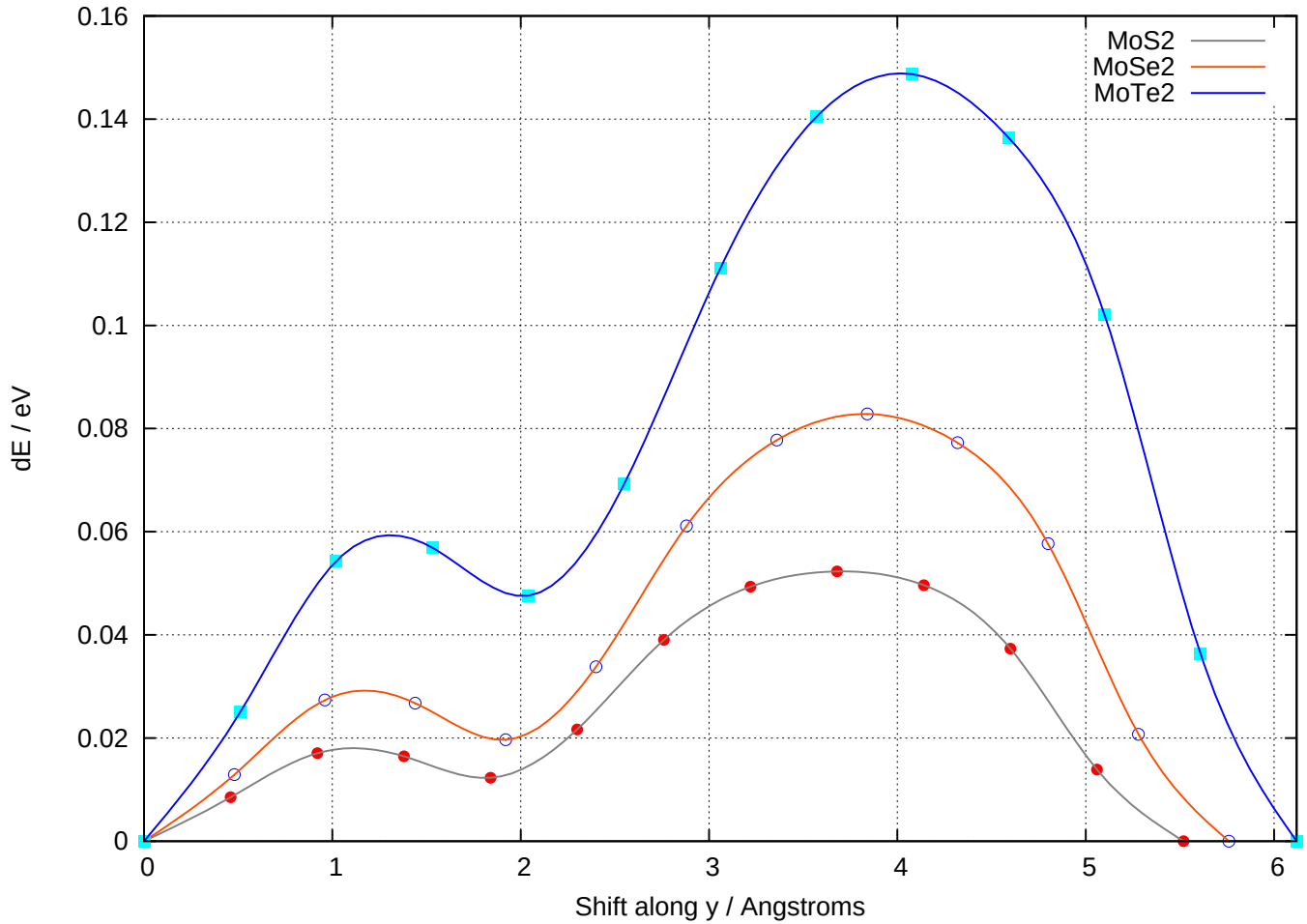


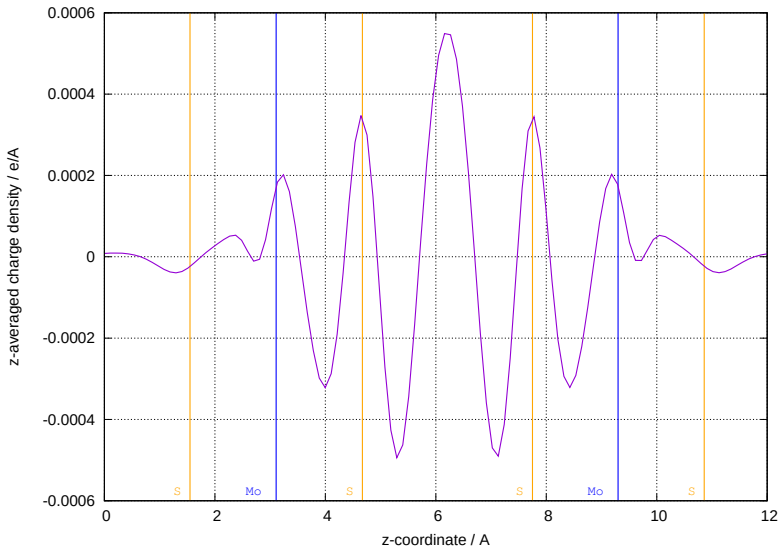
Table: Nanomechanical properties calculated for each TMD bilayer

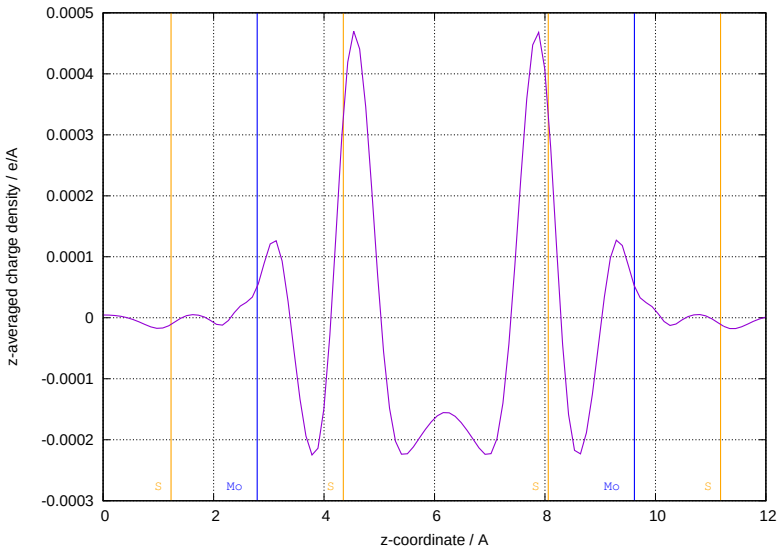
TMD	E_{bind} / meV (per cell)	γ/Jm^{-2}	f_{max} / eV/Å	τ_y/GPa
MoS_2	149.058	0.271	0.037738	0.6853
$MoSe_2$	218.230	0.366	0.056833	0.9536
$MoTe_2$	332.902	0.493	0.081934	1.2145
WS_2	267.337	0.490	0.064125	1.1748
WSe_2	333.132	0.559	0.081275	1.3631
WTe_2	440.756	0.657	0.099769	1.4874

- $E_{bind} = E_{bi} - (2 \times E_{mono})$
- $\gamma = E_{bind}/A$
- $f_{max} = dE/dy$
- $\tau_y = f_{max}/A$

Nanoscale (DOI: 10.1039/c7nr00925a)

z-averaged charge density difference plots for MoS_2:

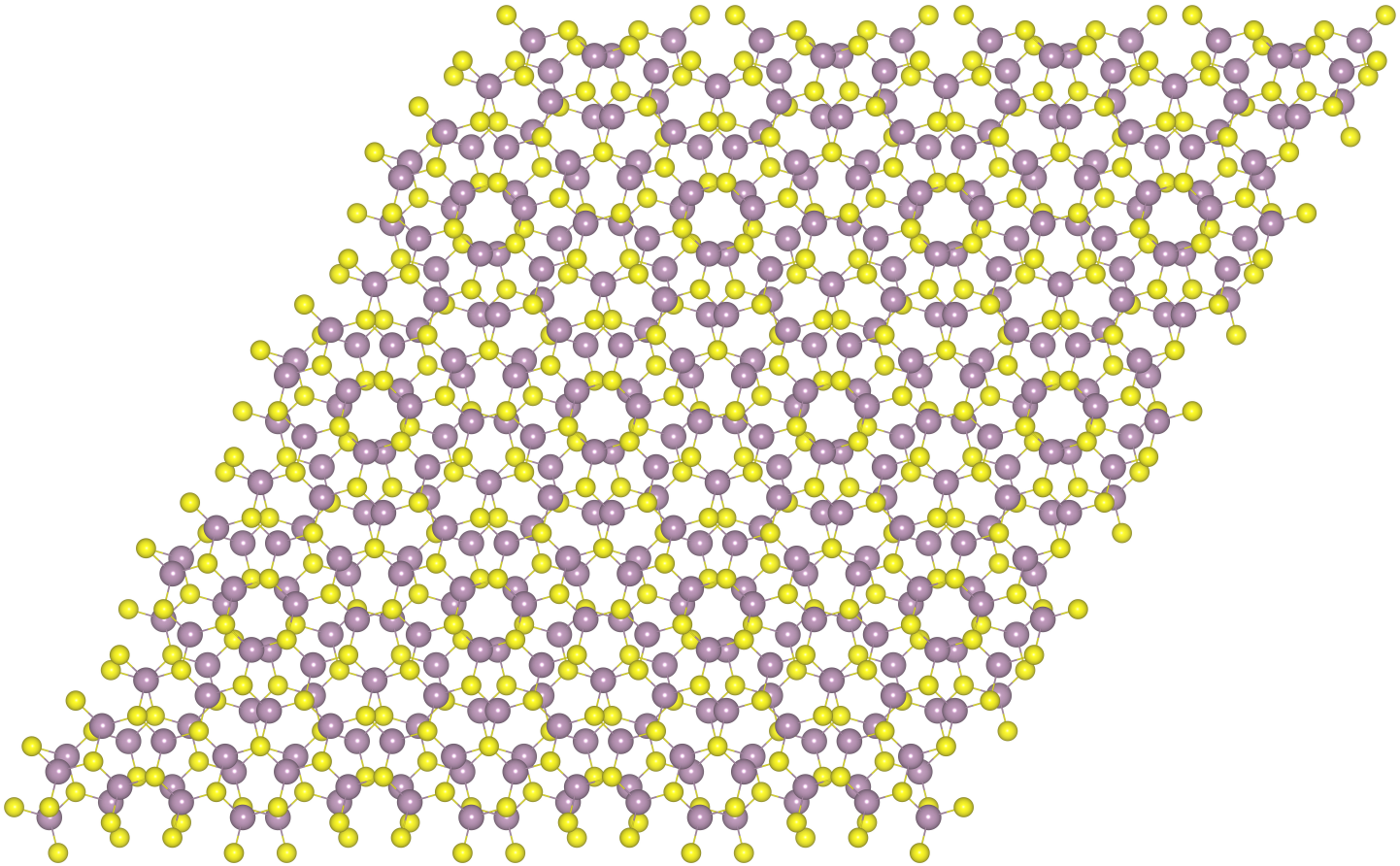




- E_{min}: charge accumulation at interface
- E_{max}: charge accumulation at chalcogens only
- Perhaps we can use fundamental properties to predict tribo behaviour...
- $\chi_{Mo} = 2.16, \chi_{W} = 2.36; \chi_{S} = 2.58, \chi_{Se} = 2.55, \chi_{Te} = 2.10$

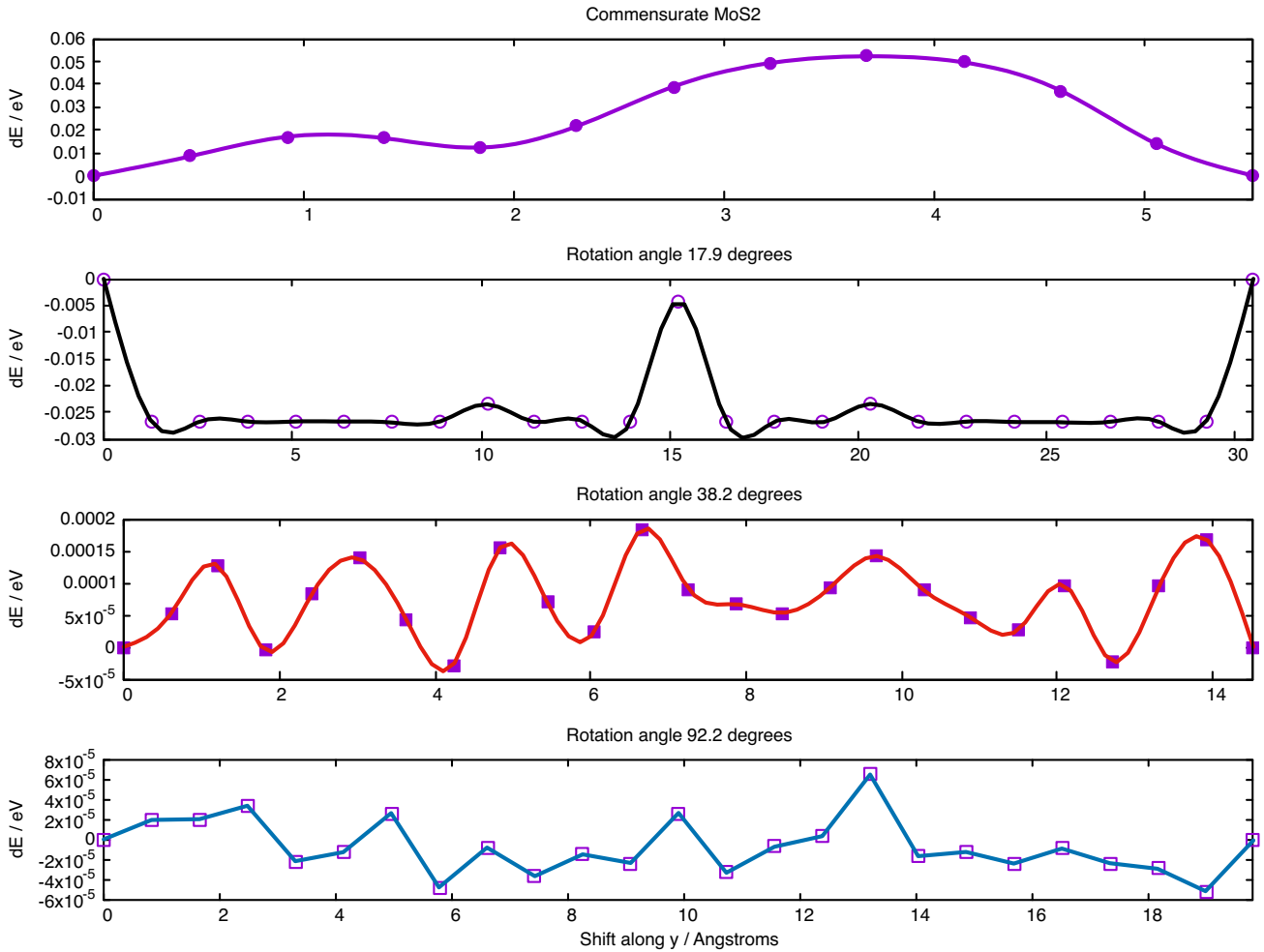
Nanoscale (DOI: 10.1039/c7nr00925a)

Top-down projection of ~~incommensurate~~ *accidentally commensurate* MoS_2 bilayer (top layer rotated 92.2° about *z*-axis):



Nanoscale (DOI: 10.1039/c7nr00925a)

The effect(s) of incommensuration have also been studied for MoS_2; it is shown that a greater degree of incommensuration results in a significant drop in calculated values of τ_y (*i.e.*, easier inter-plane shear)



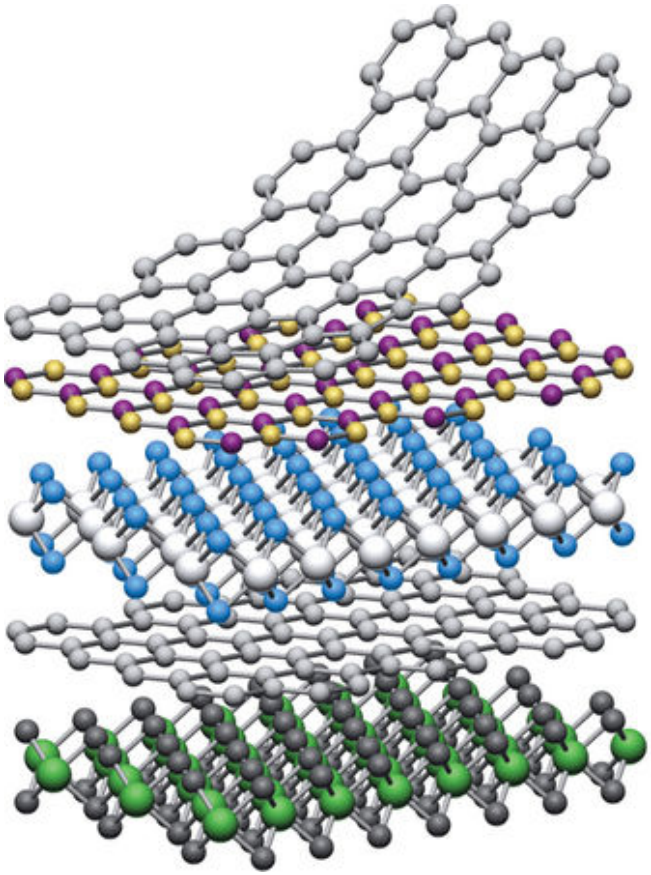
Nanoscale (DOI: 10.1039/c7nr00925a)

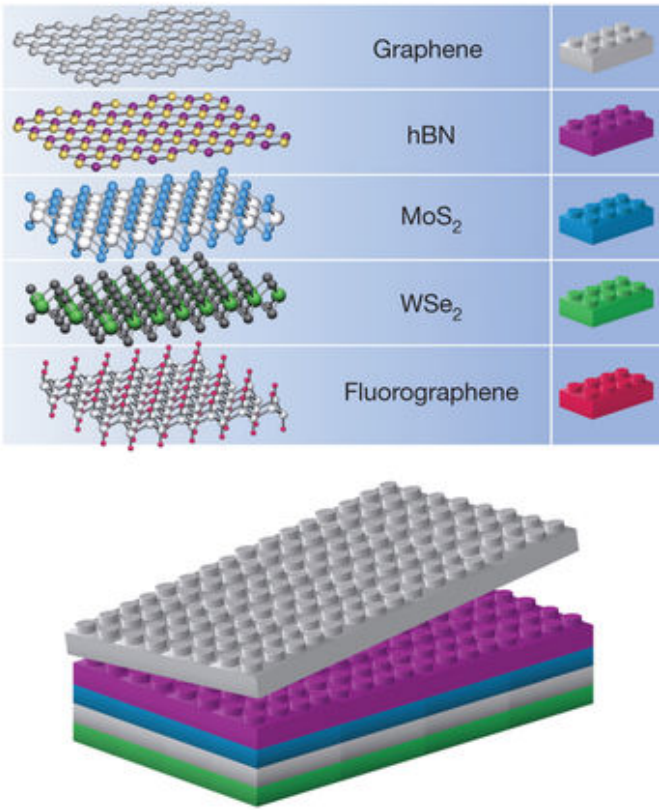
Again using the PES we can calculate the *ideal shear strength*, τ_y, for which a lower value indicates easier sliding:

Table: Nanomechanical properties calculated for each of the (in)commensurate MoS_2 bilayers

Angle of Rotation	E_{bind} / meV (per MoS_2)	γ/Jm^{-2}	f_{max} / eV/Å	τ_y/GPa
0.00	74.529	0.271	0.037738	0.6853
17.9	57.131	0.212	0.008902	0.0127
38.2	58.757	0.218	0.000105	0.0008
92.2	58.849	0.218	0.000043	0.0001

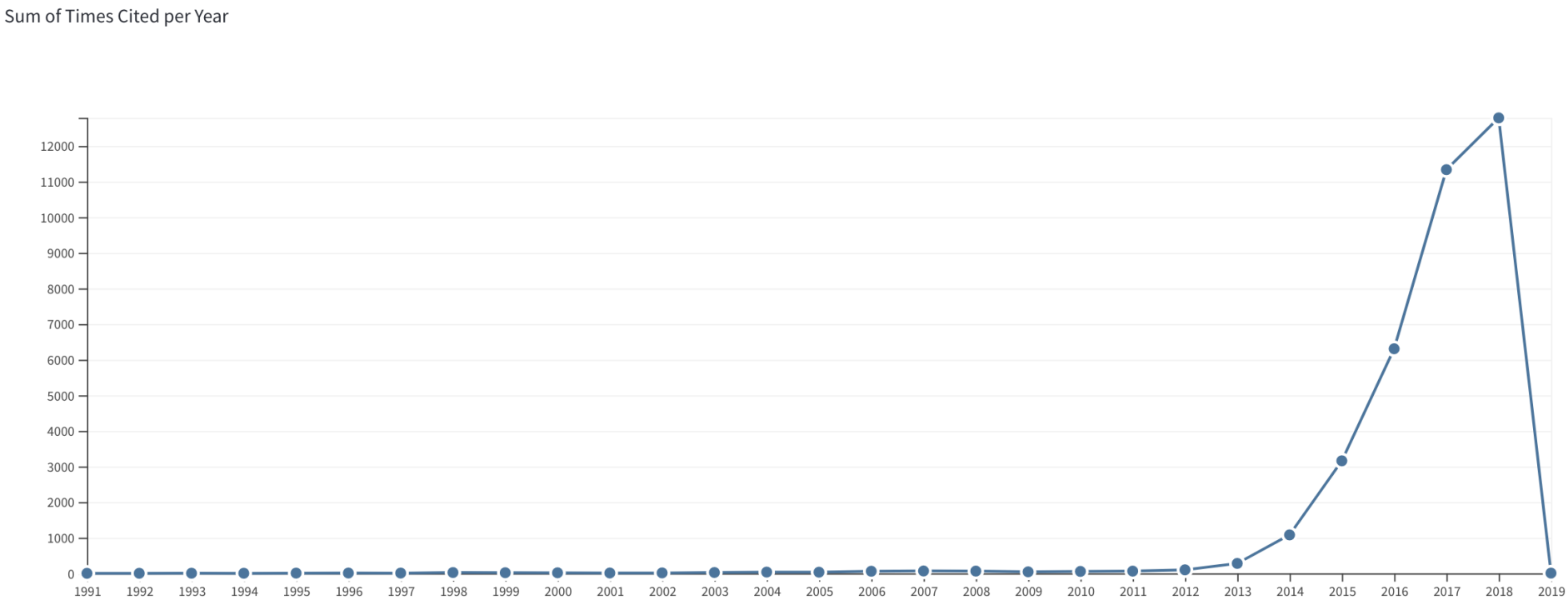
Van der Waals Heterostructures



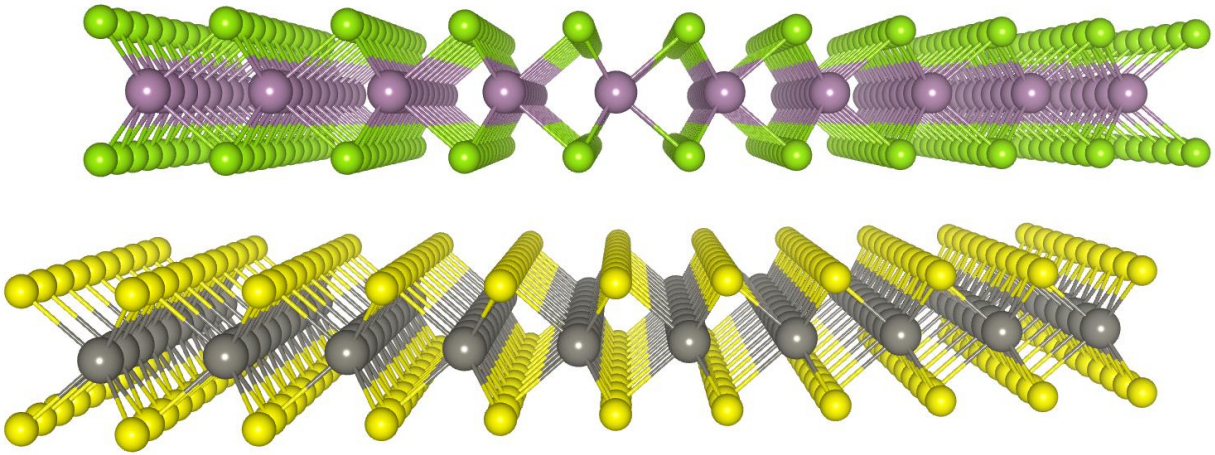


Van der Waals Heterostructures

WOS search results “van der Waals heterostructures”:



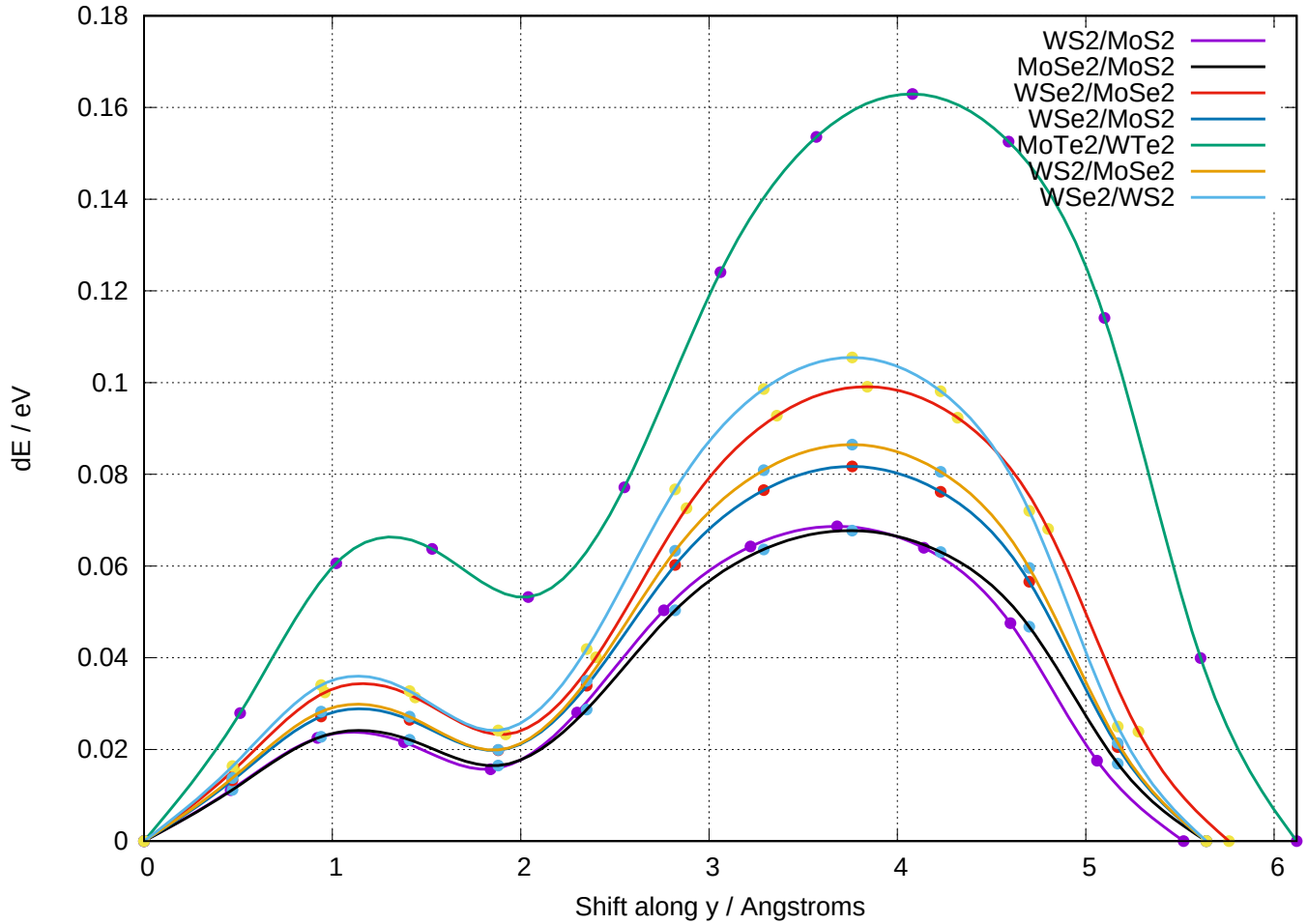
Van der Waals Heterostructures



MoSe2-on-WS2 vdwH

- Can offer excellent semiconducting properties and strong-light matter interactions
  - Power conversion efficiency enhancers
  - Photoactive layer
- Scalable fabrication still a big obstacle
  - Require sound understanding of nanomechanical properties. . .

Van der Waals Heterostructures - PES calculations



Van der Waals Heterostructures - PES calculations

TMD	E_{bind} / meV (per cell)	γ / Jm^{-2}	f_{max} / eV/Å	τ_y / GPa
MoS_2	149.058	0.271	0.037738	0.6853
$MoSe_2$ || MoS_2	182.161	0.319	0.046099	0.8065
WS_2 || MoS_2	198.755	0.362	0.048498	0.8830
$MoSe_2$	218.230	0.366	0.056833	0.9536
WSe_2 || MoS_2	225.831	0.394	0.055964	0.9775
WS_2 || $MoSe_2$	240.856	0.421	0.060308	1.0546
WSe_2 || $MoSe_2$	268.694	0.449	0.067703	1.1326
WS_2	267.337	0.490	0.064125	1.1748
$MoTe_2$	332.902	0.493	0.081934	1.2145
WSe_2 || WS_2	300.199	0.524	0.074150	1.2946
$MoTe_2$ || WTe_2	381.674	0.563	0.092021	1.3571
WSe_2	333.132	0.559	0.081275	1.3631
WTe_2	440.756	0.657	0.099769	1.4874

- Now formulating relationship between electronic properties of vdwH systems and nanomechanical properties

Acknowledgements

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Thank you for your attention