
Computational Synthesis

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Pankaj Rajak, Guoqing Zhou

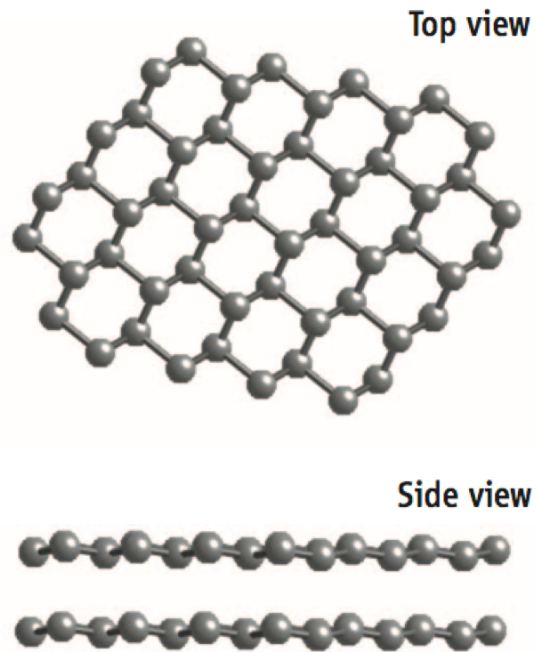


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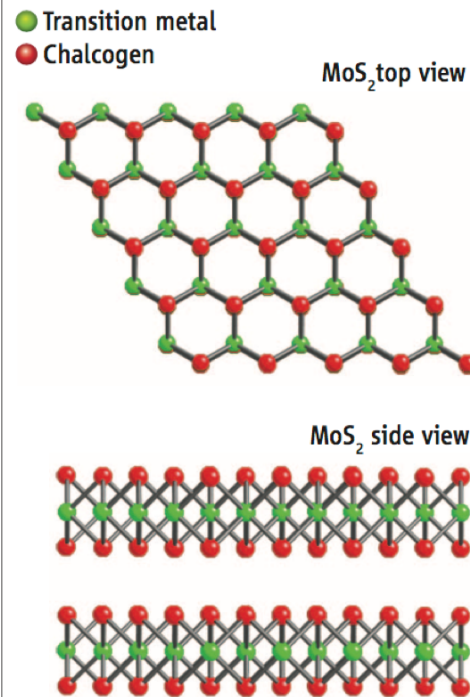
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Layered Materials

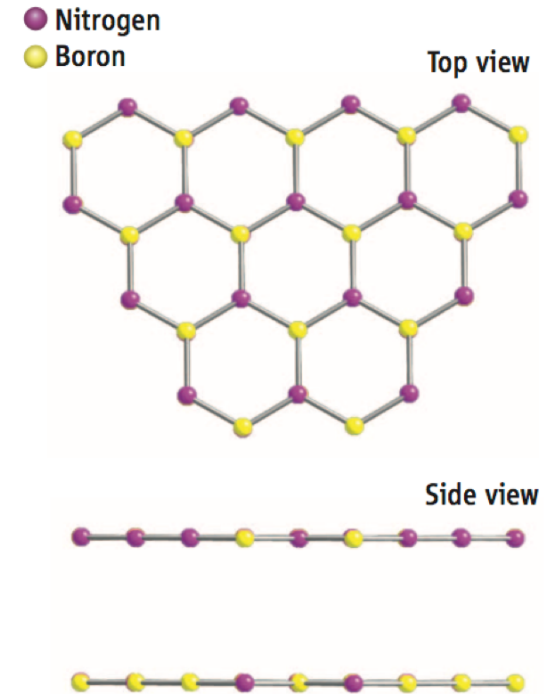
Graphene



Transition Metal Dichalcogenides



Boron Nitride



Experimental Approaches

- **Chemical Vapor Deposition**
- **Liquid-Phase Exfoliation**



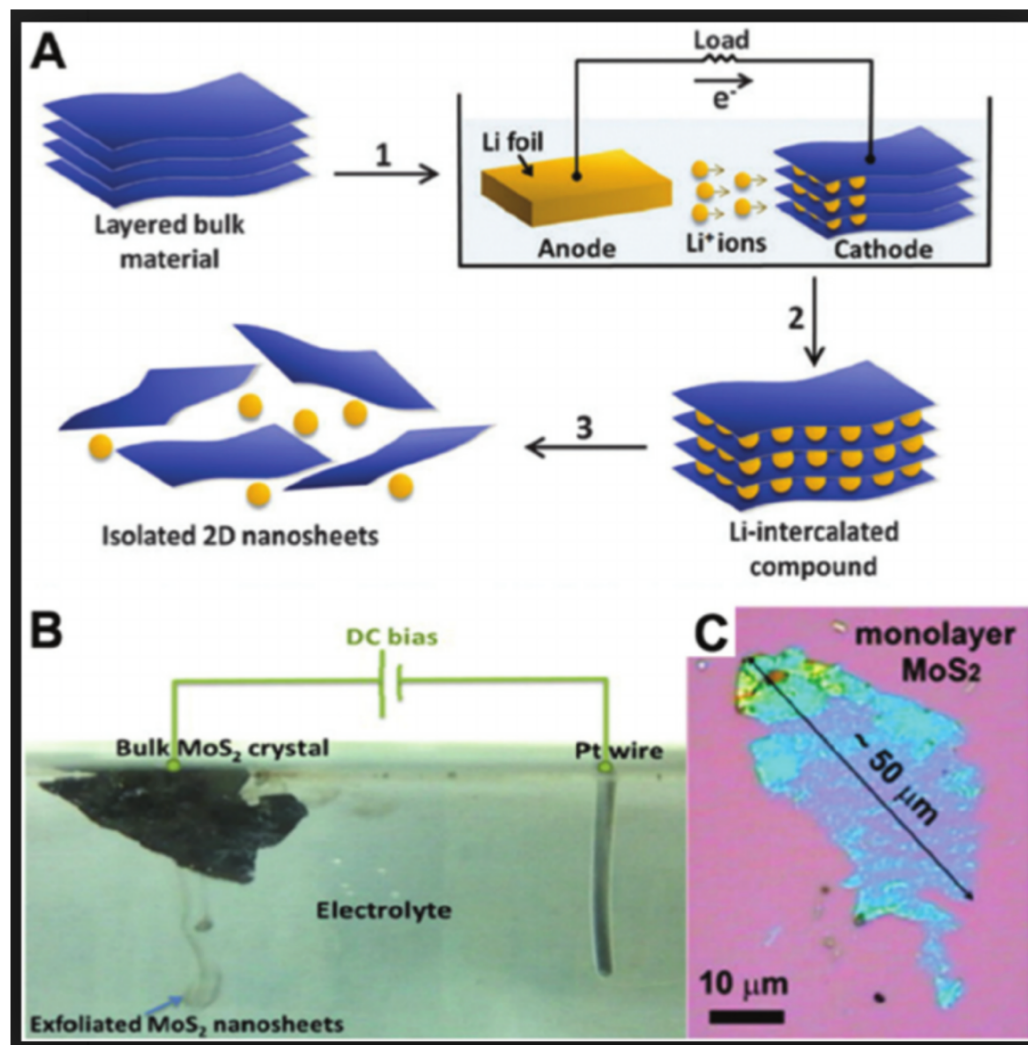
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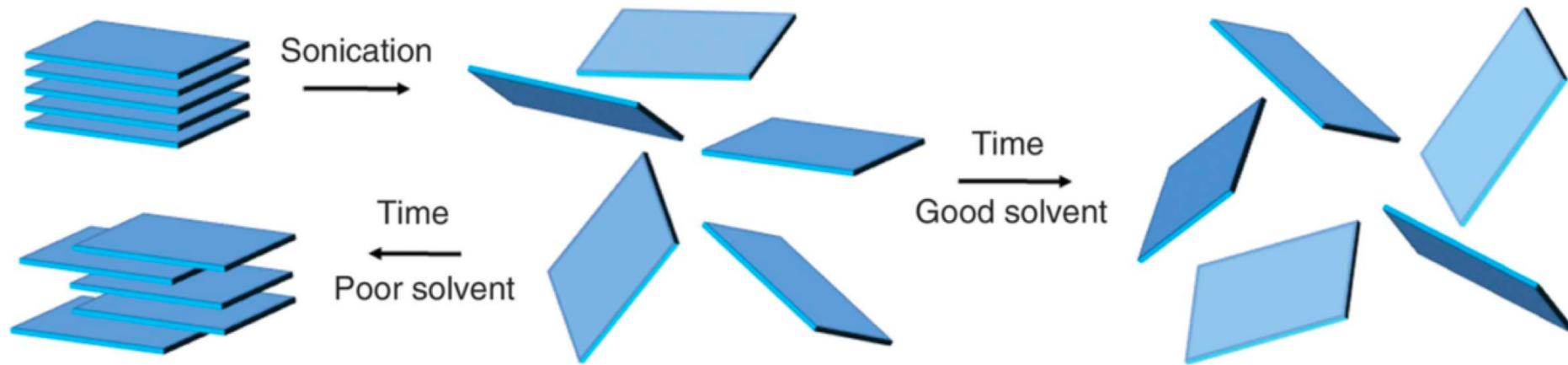
Liquid-Phase Exfoliation Approaches

- **Electrochemical**
- **Sonication**
- **Shear**

Electrochemical Exfoliation



Exfoliation by Sonication



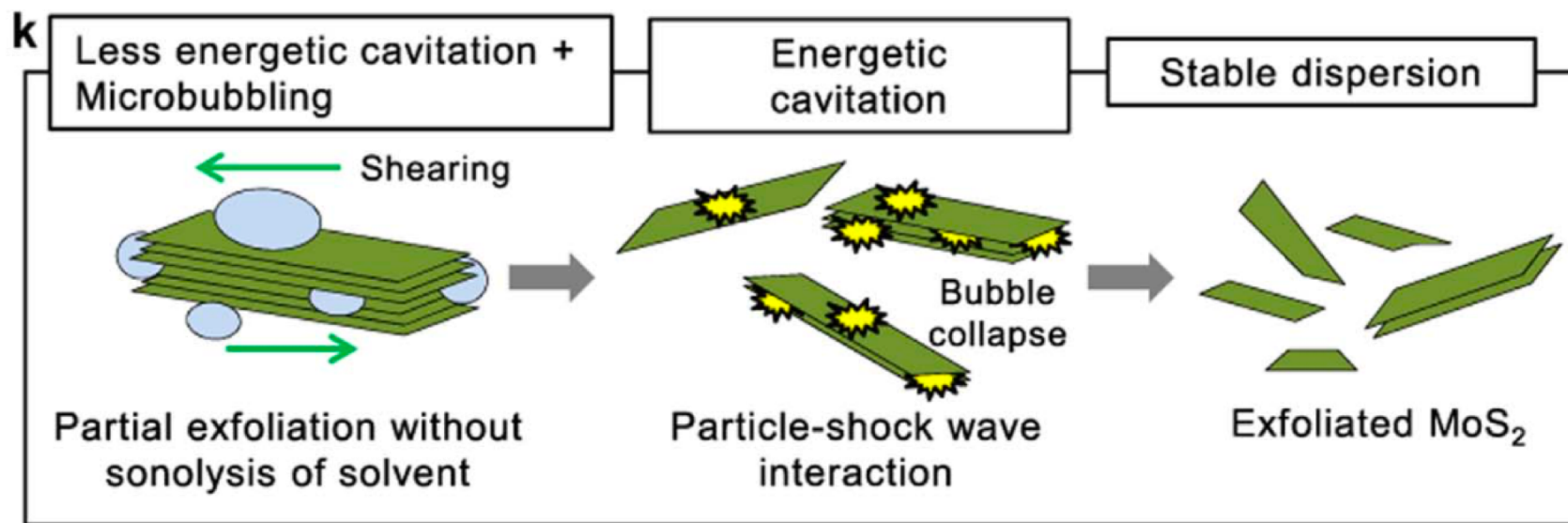
Solvent plays a critical role

Shear Exfoliation

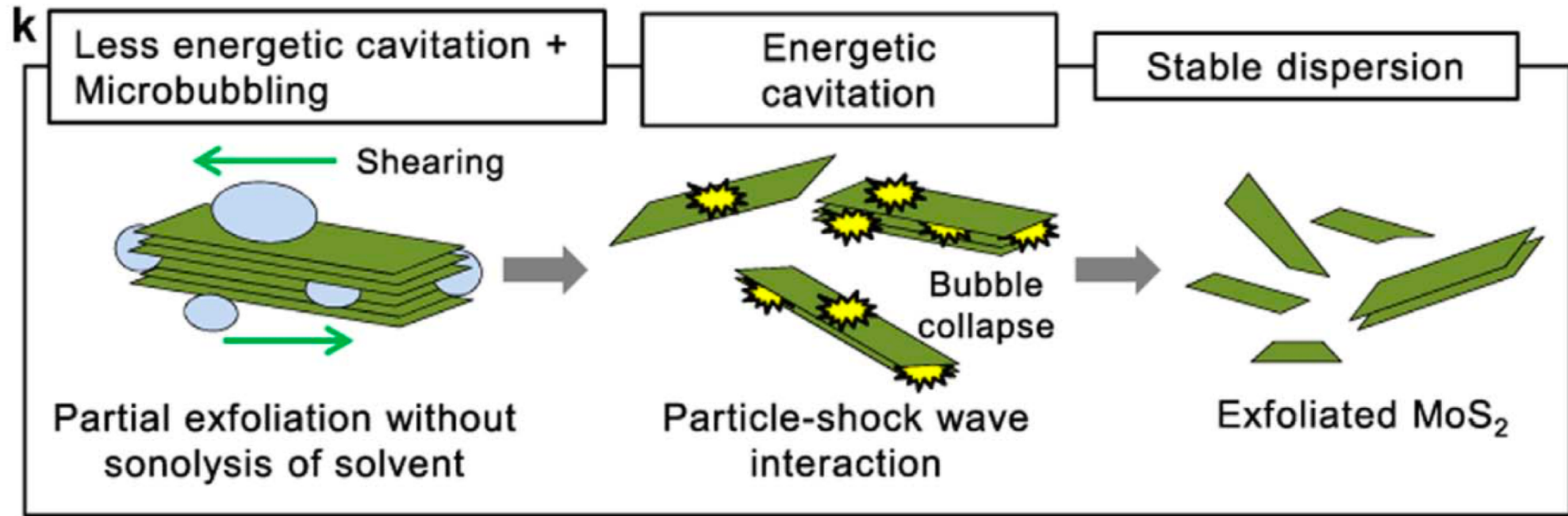
Minimum shear rate of exfoliation: $\dot{\gamma} = \frac{\sqrt{E_{S,G}} - \sqrt{E_{S,L}}}{\eta L}$

$E_{S,G}$ = surface energy of layered material; L = flake length

$E_{S,L}$ = surface energy of liquid; η = liquid viscosity



Exfoliation by Shearing & Sonication



Solvent plays a critical role

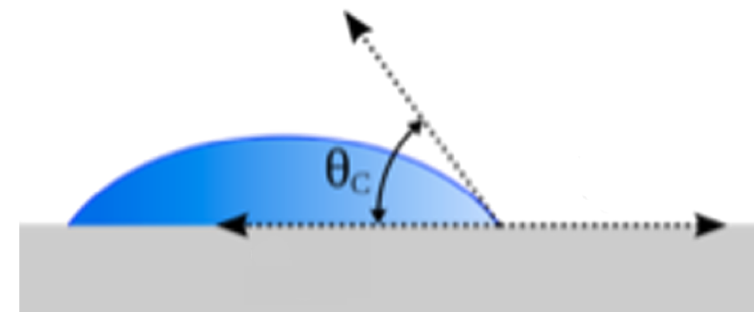
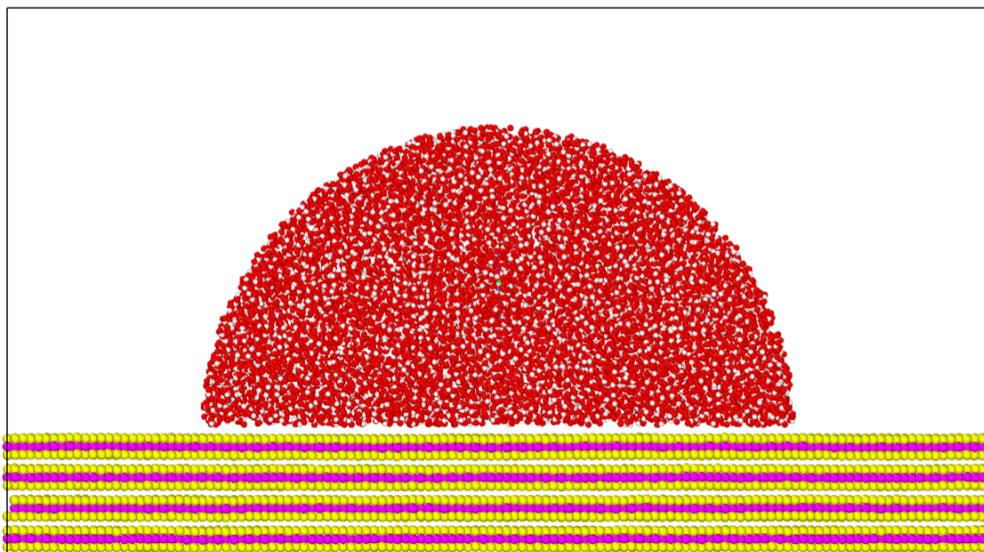
Hands-on Tutorials

- Force fields for MD simulations of exfoliation (**Guoqing Zhou**)
- Shock simulations using MD (**Pankaj Rajak**)
- MD simulations/analysis of exfoliation (**Ken-ichi Nomura**)



Force Field Development (Guoqing)

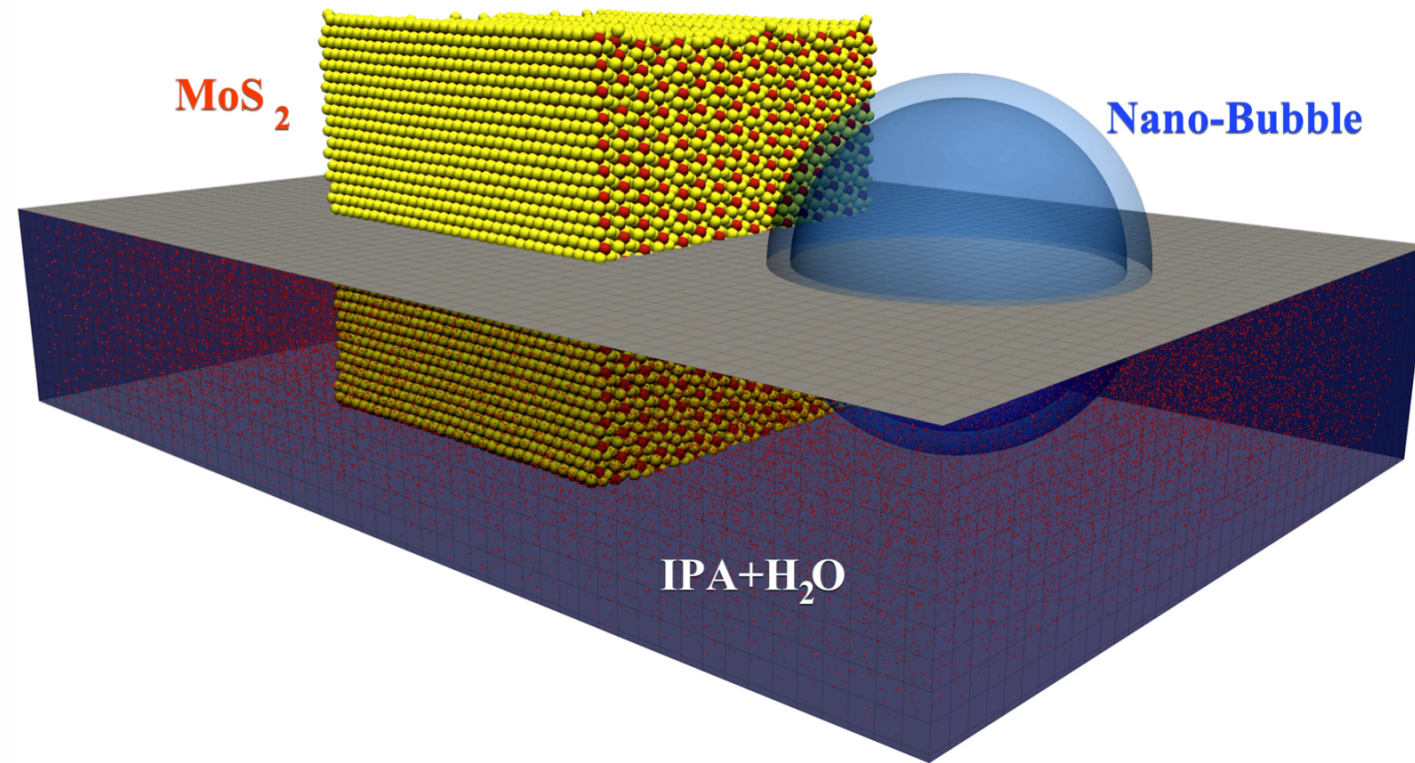
- 1) Create and relax the liquid and MoS₂ separately
- 2) Hands-on: Place liquid droplet on MoS₂ and relax the system at 25°C in NVT ensemble



Solvent

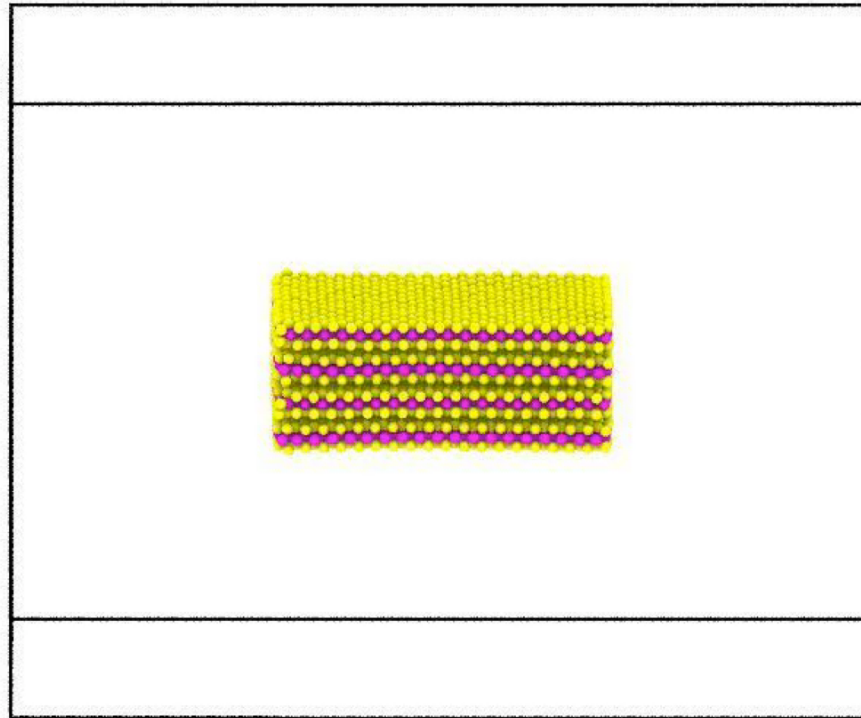
MoS₂ substrate

MD Simulation of Exfoliation (Pankaj & Ken-ichi)



MD Simulation of Shear Exfoliation

Next Workshop

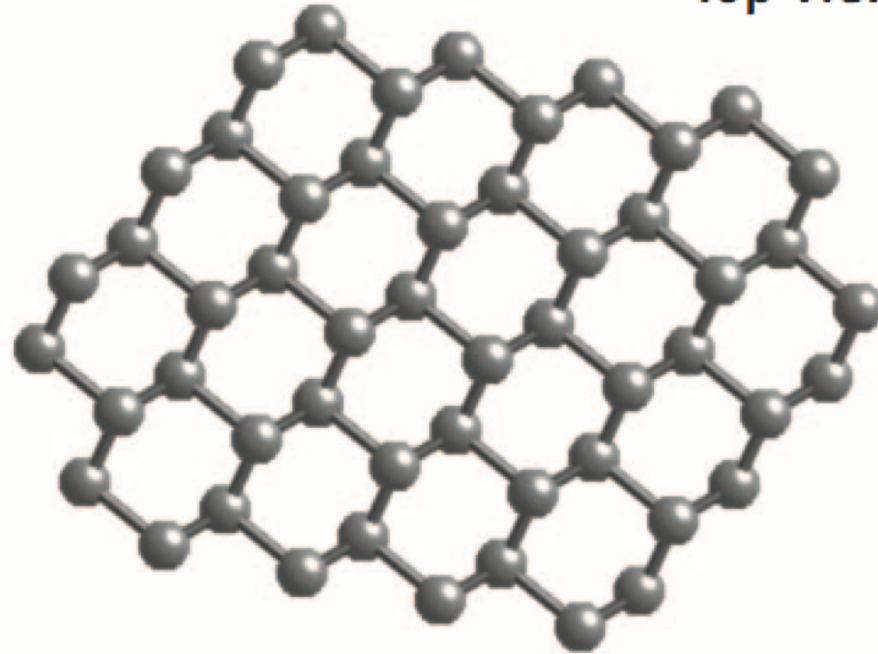


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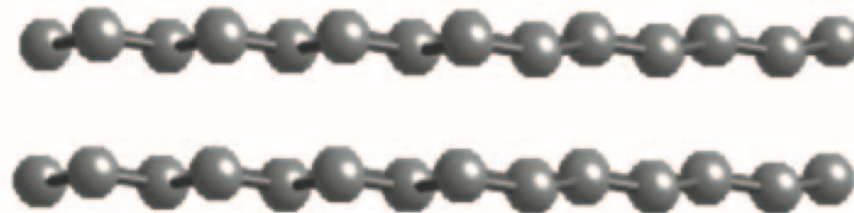


Graphene

Top view



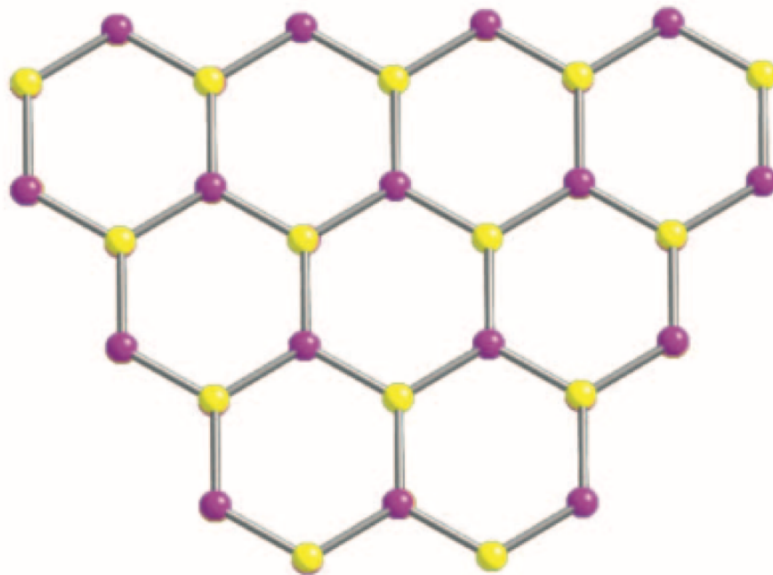
Side view



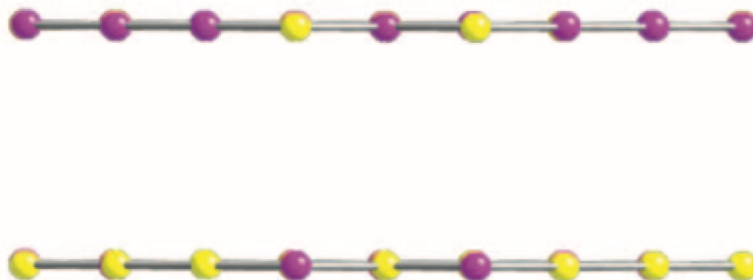
Boron Nitride (h-BN)

● Nitrogen
● Boron

Top view



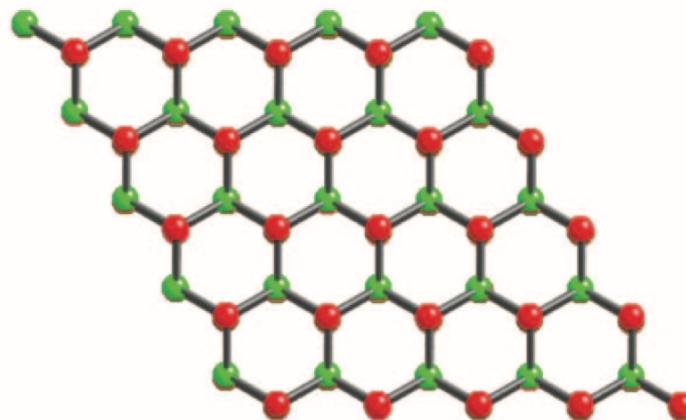
Side view



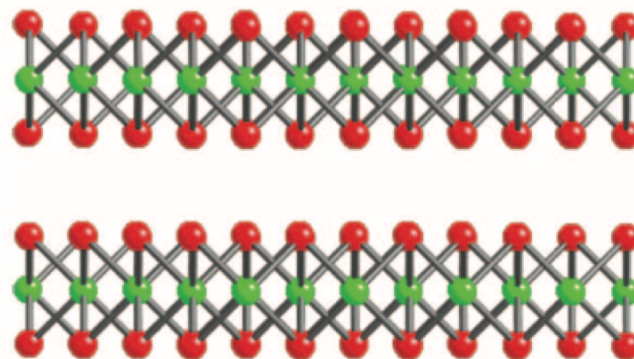
Transition Metal Dichalcogenides

- Transition metal
- Chalcogen

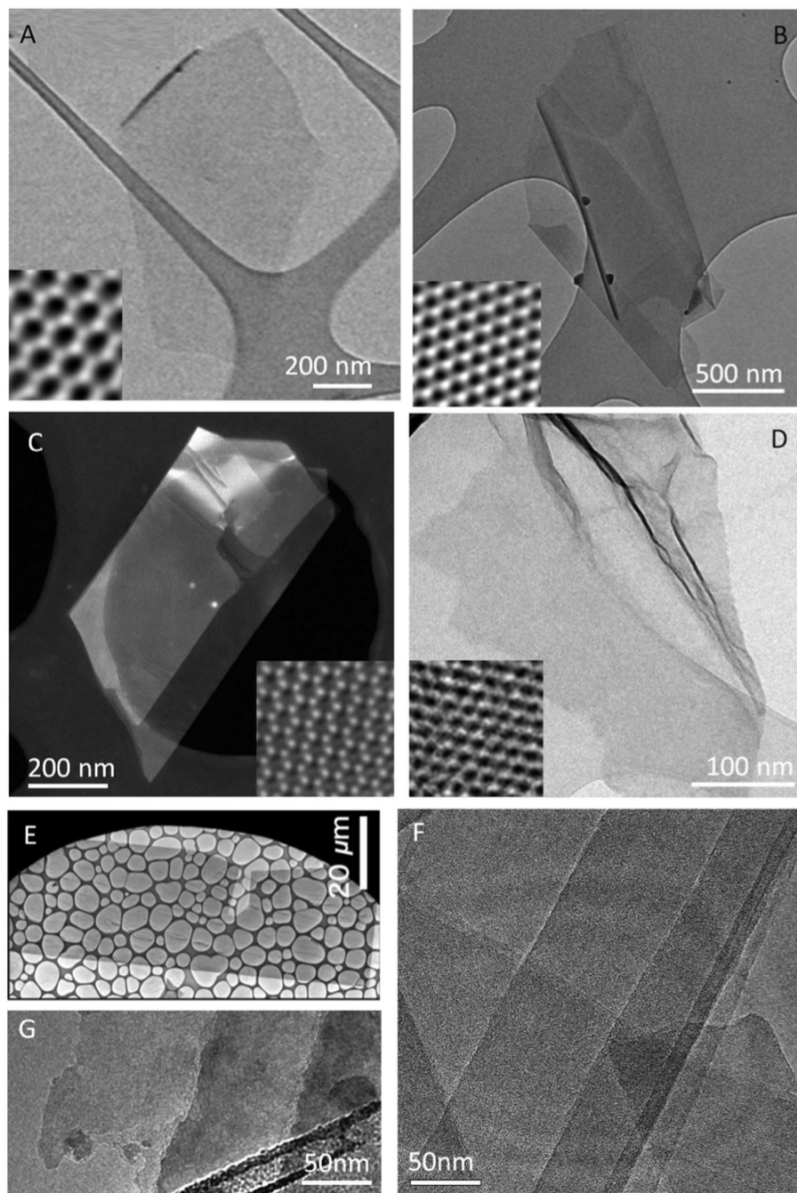
MoS₂ top view



MoS₂ side view

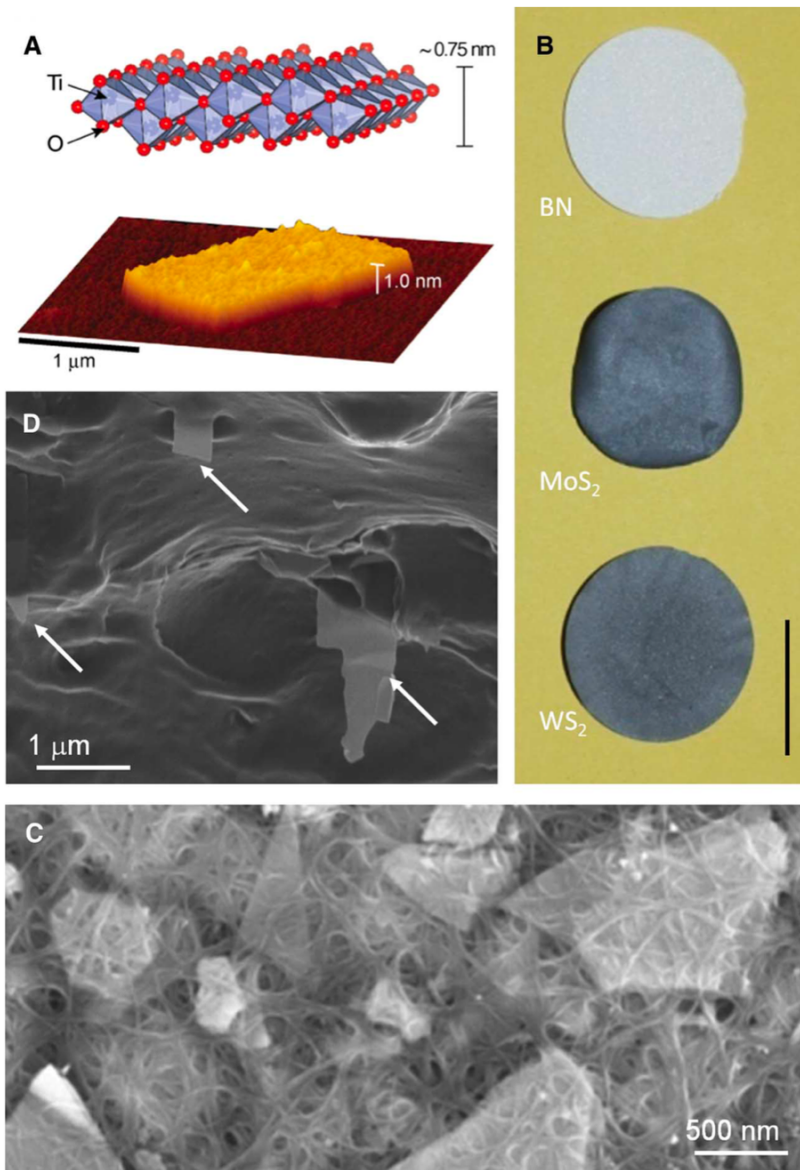


Liquid Exfoliated Nanosheets – TEM Images



- (A) Graphene nanosheet exfoliated in N-methyl-pyrrolidone.
- (B) h-BN nanosheet exfoliated in the solvent isopropanol
- (C) An MoS₂ nanosheet exfoliated an aqueous surfactant solution
- (D) An MoS₂ nanosheet exfoliated by Li ion intercalation
- (E) A TiO₂ nanosheet exfoliated by ion exchange
- (F) Functionalized layered double hydroxide nanosheets exfoliated in ethanol.
- (G) Hydroxylated metal carbide nanosheets exfoliated in methanol

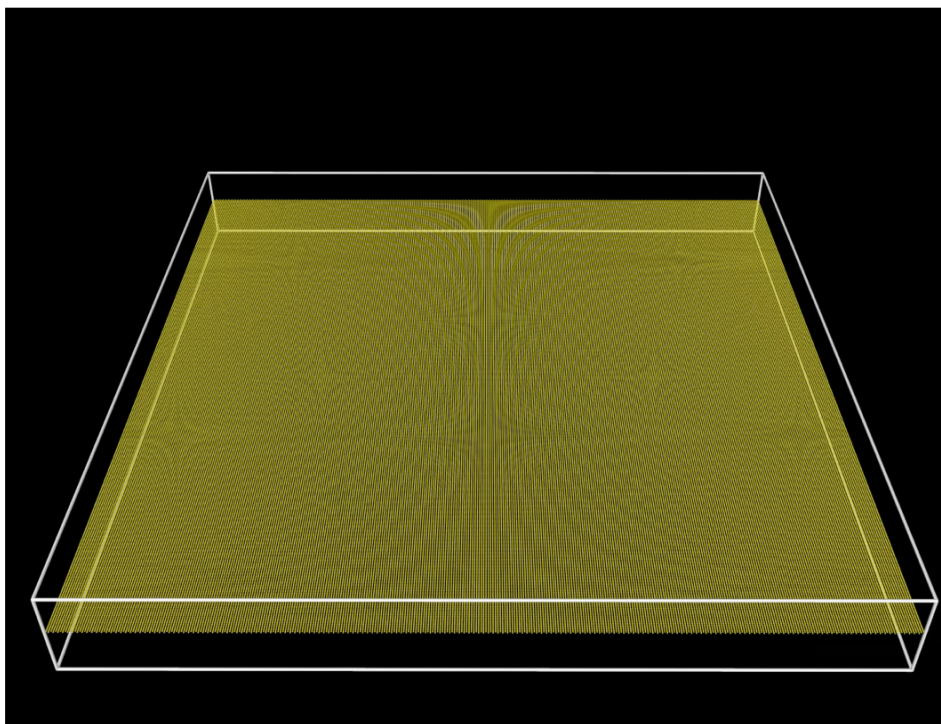
Layered Material Structures After Exfoliation



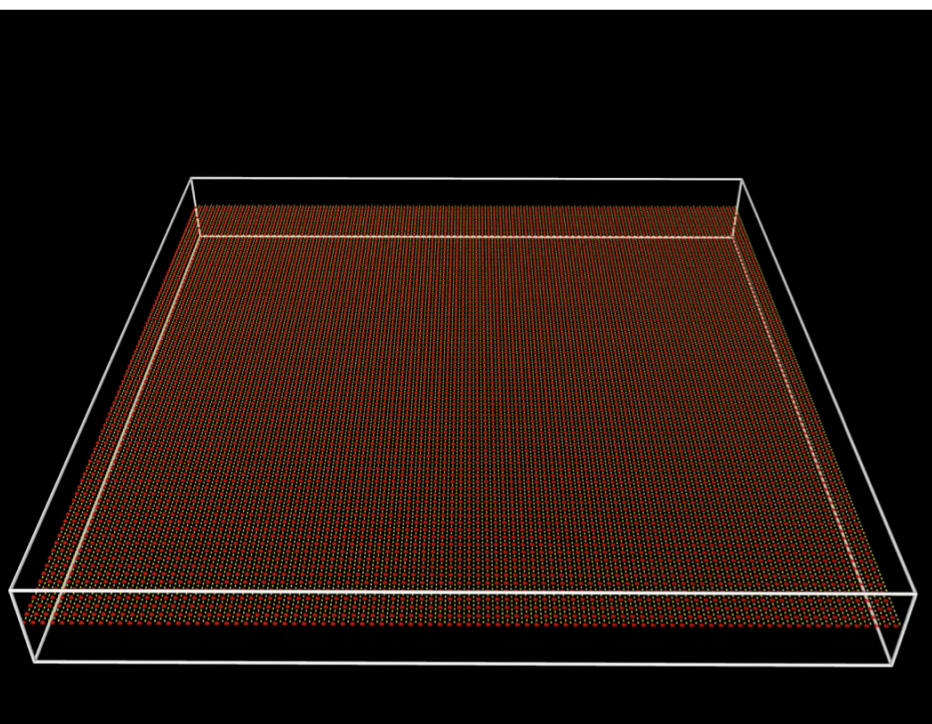
- TiO_2 nanosheets deposited onto a substrate and imaged by AFM.
- Solution-processed, free-standing films of randomly arranged nanosheets of h-BN, MoS_2 , and WS_2 . Scale bar, 25 mm.
- A composite film of WS_2 nanosheets in a matrix of randomly arranged CNTs
- Solvent-exfoliated graphene nanosheets (arrows) embedded in a polymer matrix

Dewetting Transition in MoS₂ bilayer

H₂O monolayer



H₂O/IPA monolayer



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