

# A Rigorous Method of Calculating Exfoliation Energies from First Principles

## Current Topic: Thermal Properties of Copper Halides

---

Previous: Jong Hyun Jung,<sup>1</sup> Cheol-Hwan Park,<sup>1</sup> and Jisoon Ihm<sup>2</sup> Nano Lett. 18, 2759 (2018).

1) Department of Physics and Astronomy, Seoul National University, Korea

2) Department of Physics, Pohang University of Science and Technology, Korea

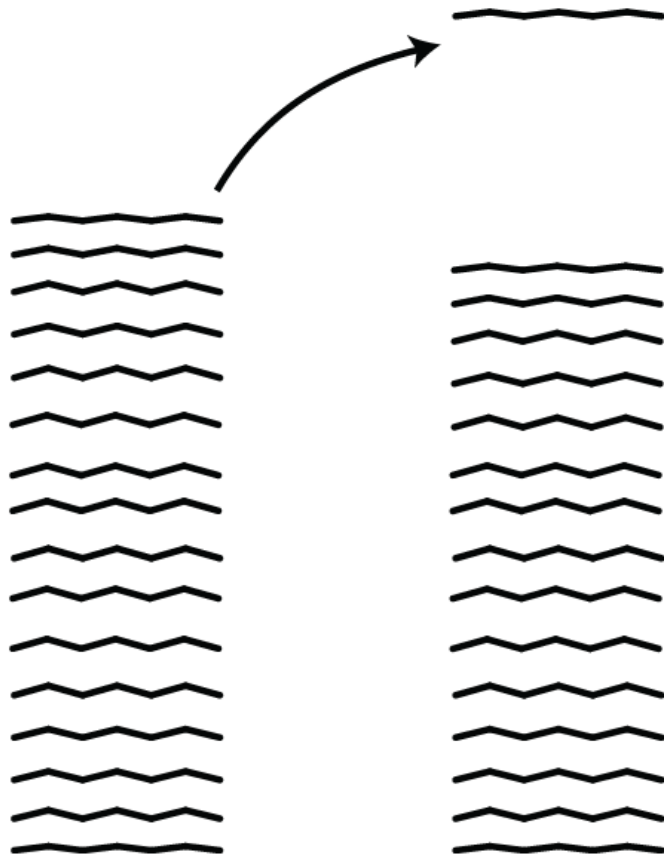
Current: with Christian Carbogno, Matthias Scheffler

May 13, 2019, Coffee talk

# Significance of Exfoliation Energy

---

Exfoliation energy



Why some 2D materials are easily exfoliated?

Which 2D materials can be obtained from mechanical exfoliation in the future?

# Gap

---

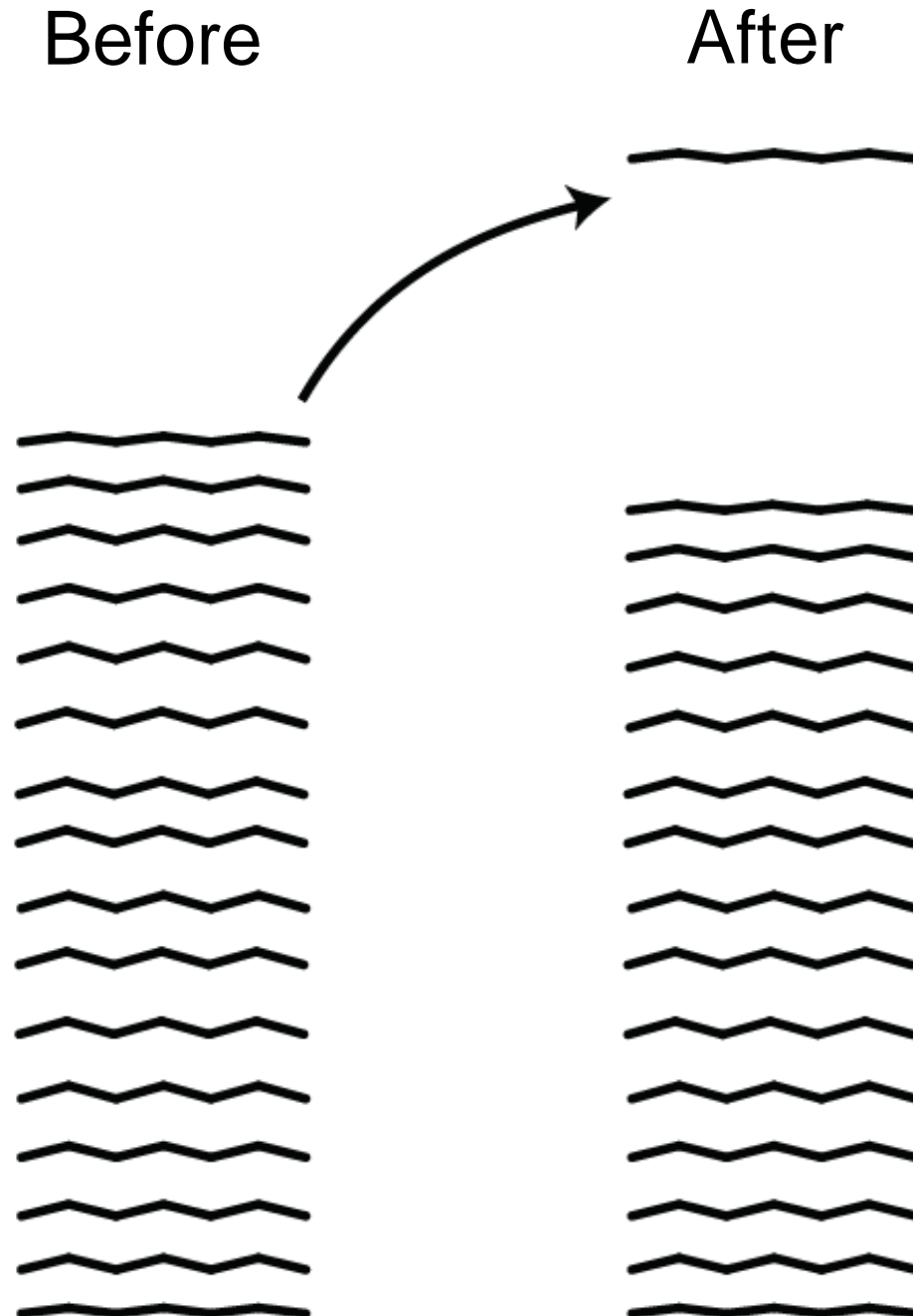
Traditional calculation method

- $E(\text{After}) - E(\text{Before})$

Heavy computation

- Many layers to mimic an infinitely thick slab
- Convergence with respect to the number of layers

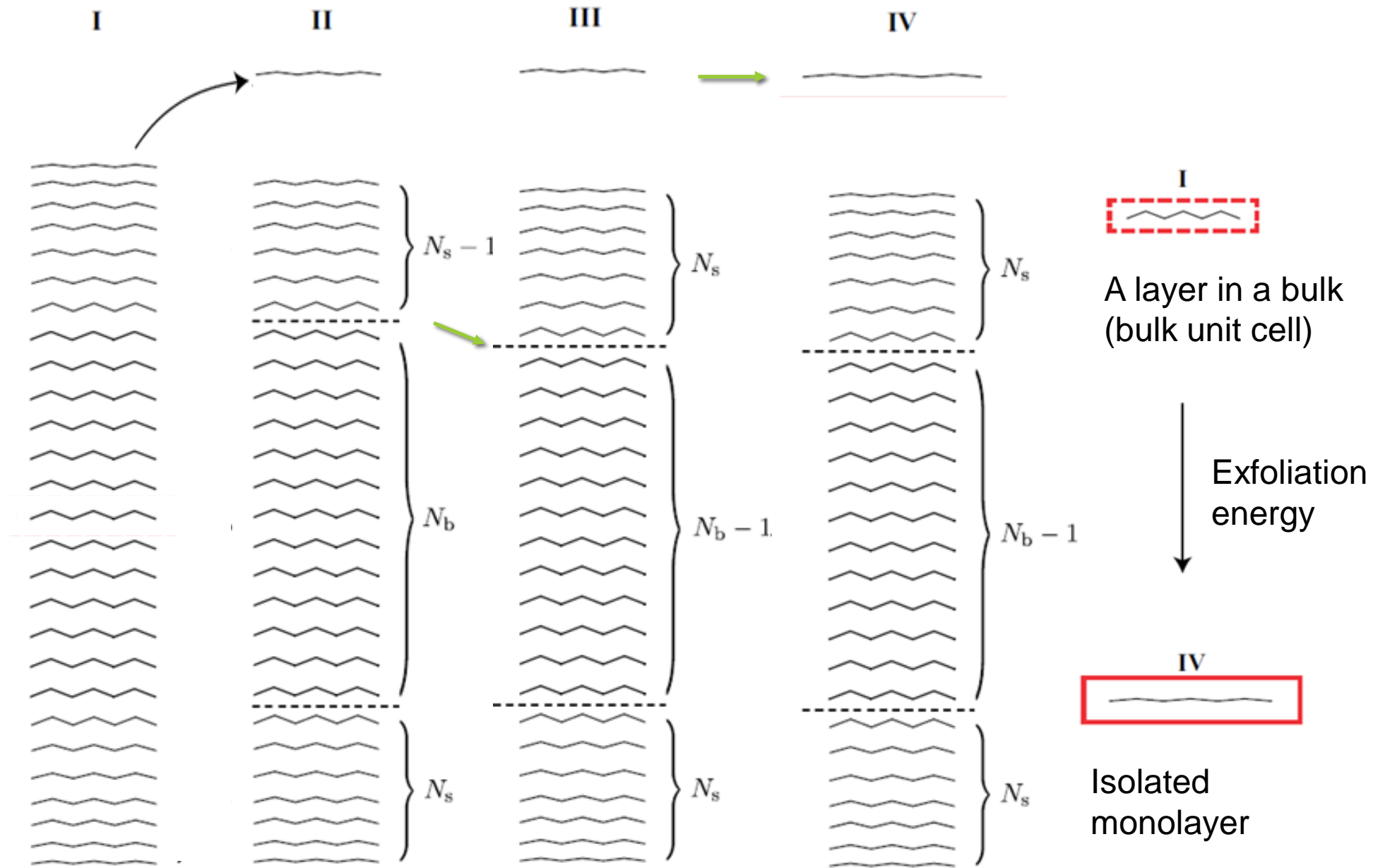
Cannot account for surface reconstructions



# Our Method

Exfoliation energy  
= Energy difference  
between an isolated  
single layer, and a  
layer in a bulk

Very efficient



# *n*-layer Exfoliation Energy

---

## Extension

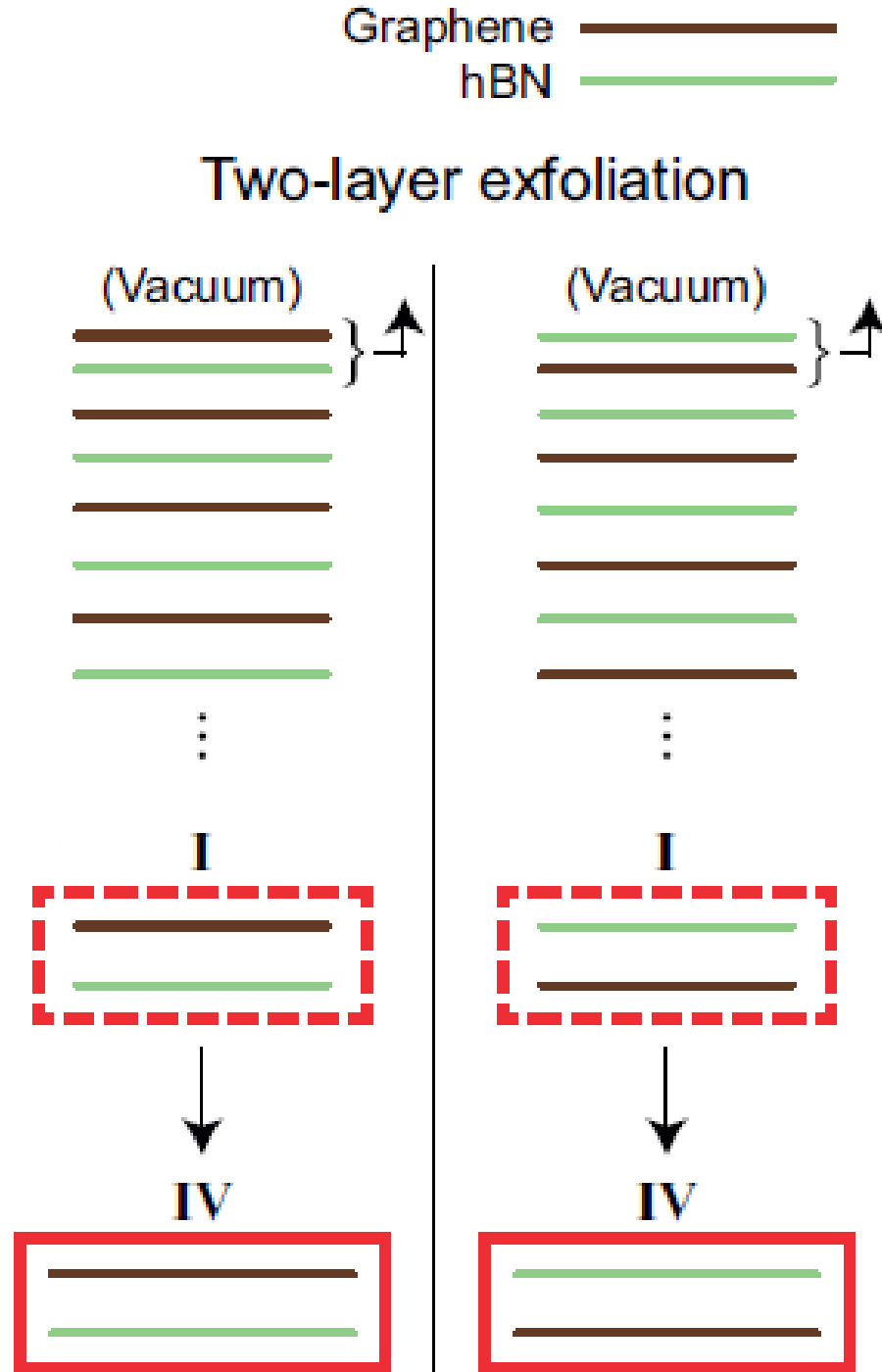
*n*-layer exfoliation energy: Energy cost to separate *n* layers simultaneously

The exfoliation energy is obtained as the energy difference between separated *n* layers, and *n* layers in the bulk.

# Two-layer Exfoliation

Here, our method does not apply to the one-layer exfoliation energy, but that of two layers.

The left and right structures have the same exfoliation energies.

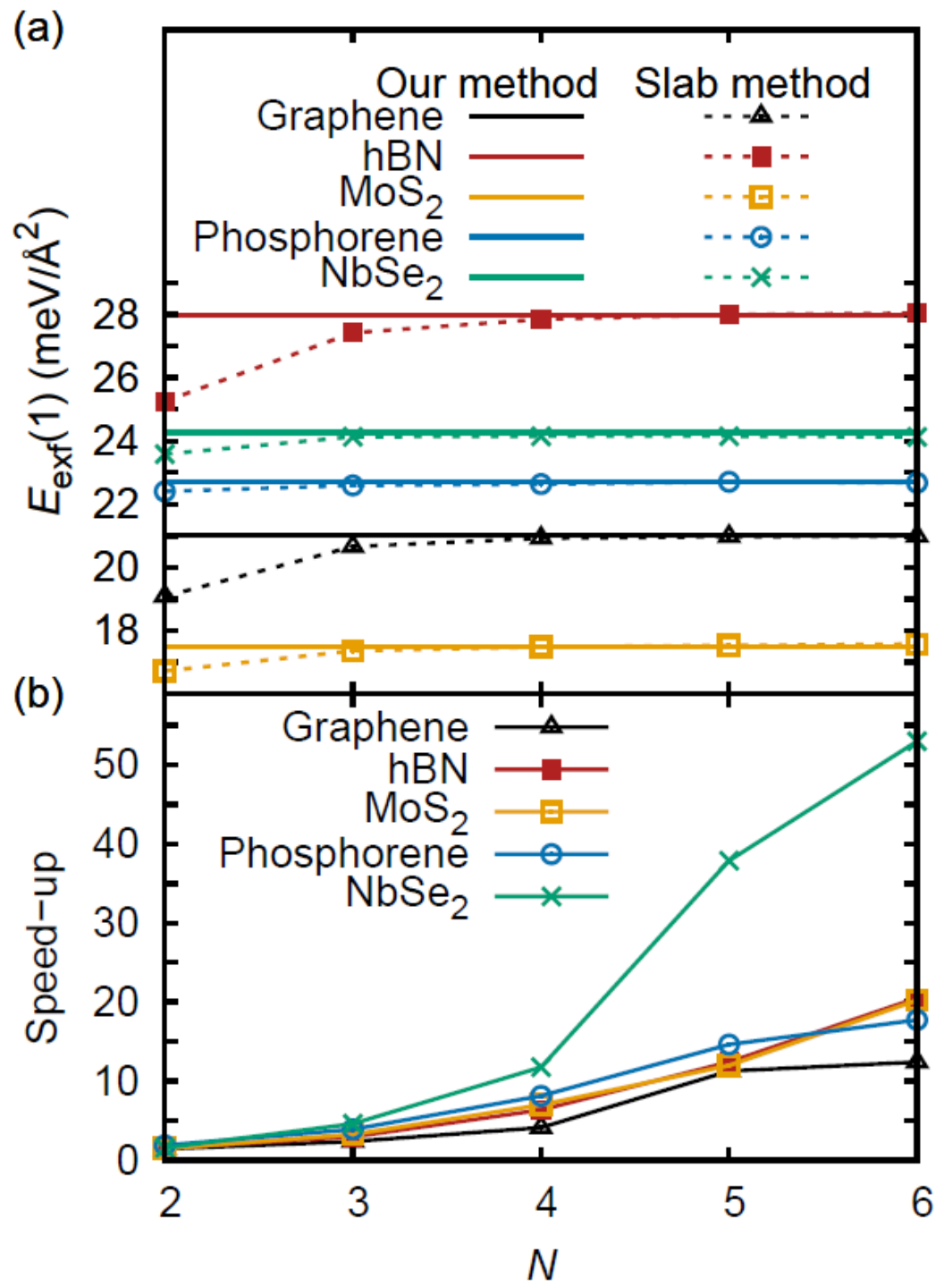


# Demonstration of Our Method

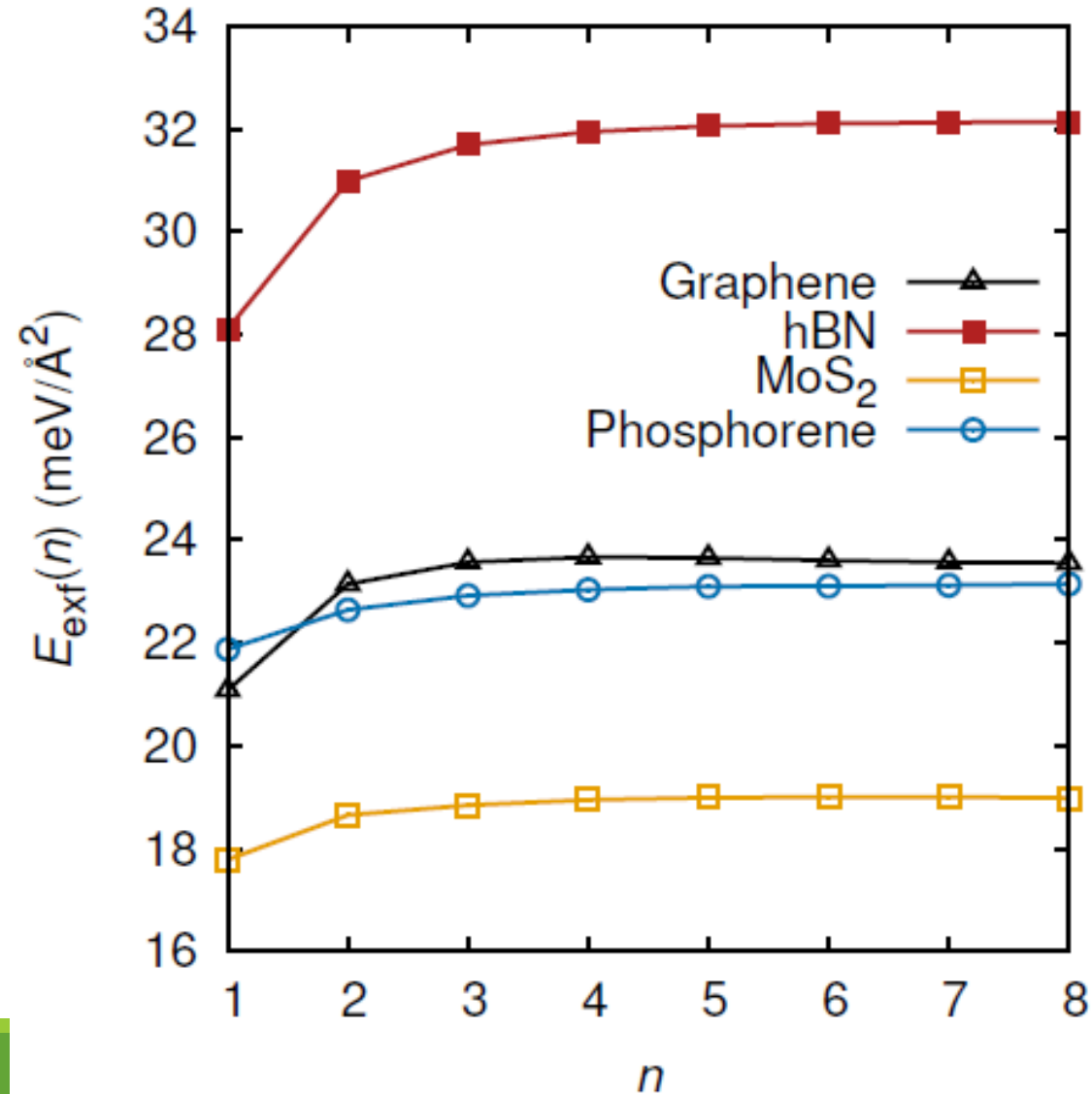
Density-functional theory

Monolayer exfoliation energy using the traditional method on an  $N$ -layer slab converges to the value from our method.

Huge speed-up

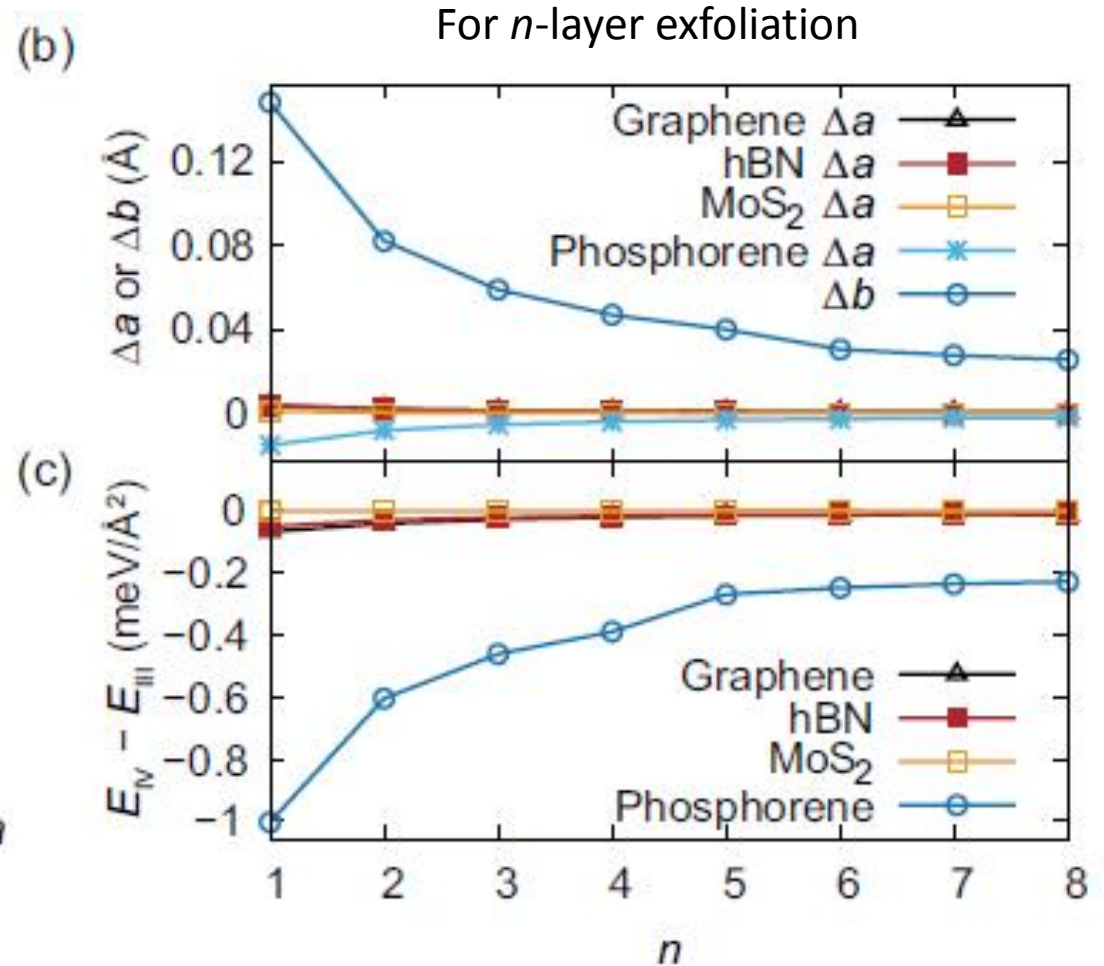
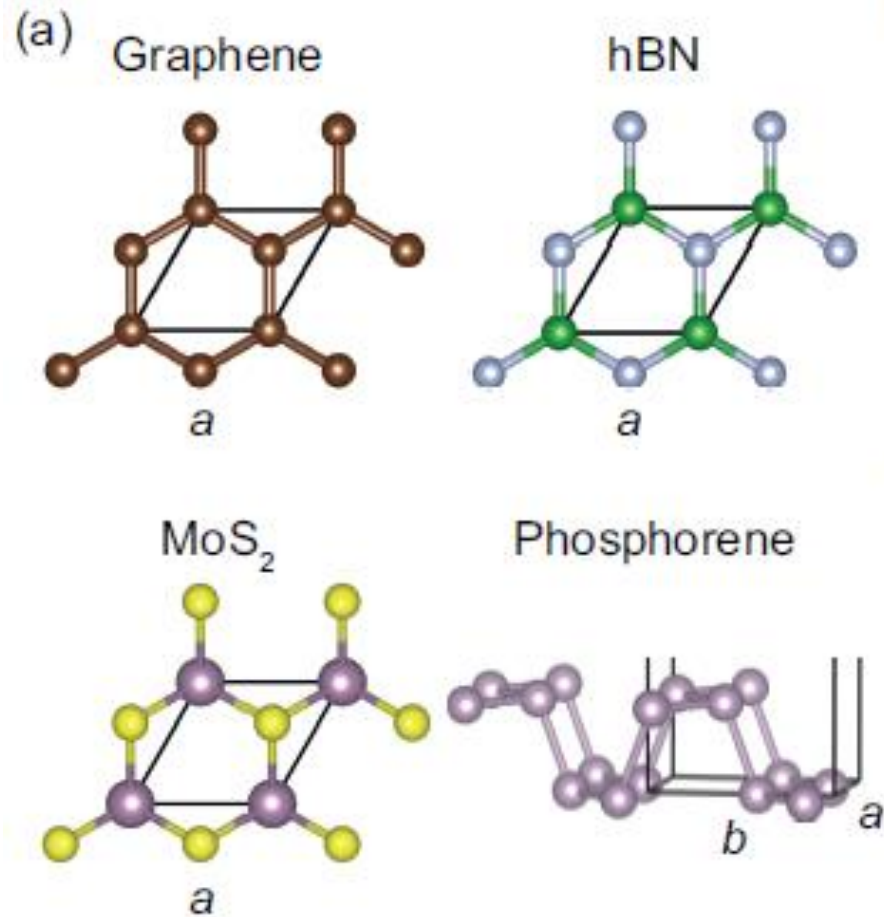


# $n$ -layer Exfoliation Energy: Our Method



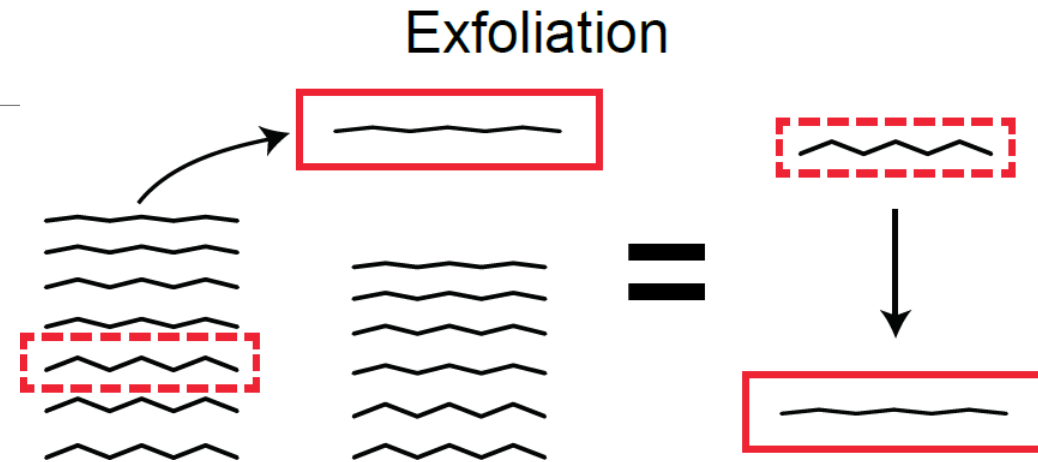


# The Exfoliated Layer Expands



# Summary

---



## Pros

- ❖ Rigorous
- ❖ Significant efficiency
- ❖ Generally applicable
- ❖ In-plane lattice parameters
- ❖ Surface reconstructions

## Cons

Periodic  
boundary  
condition