

# First-Principles Multiscale Modeling Enabled by Machine-Learning Interatomic Potentials

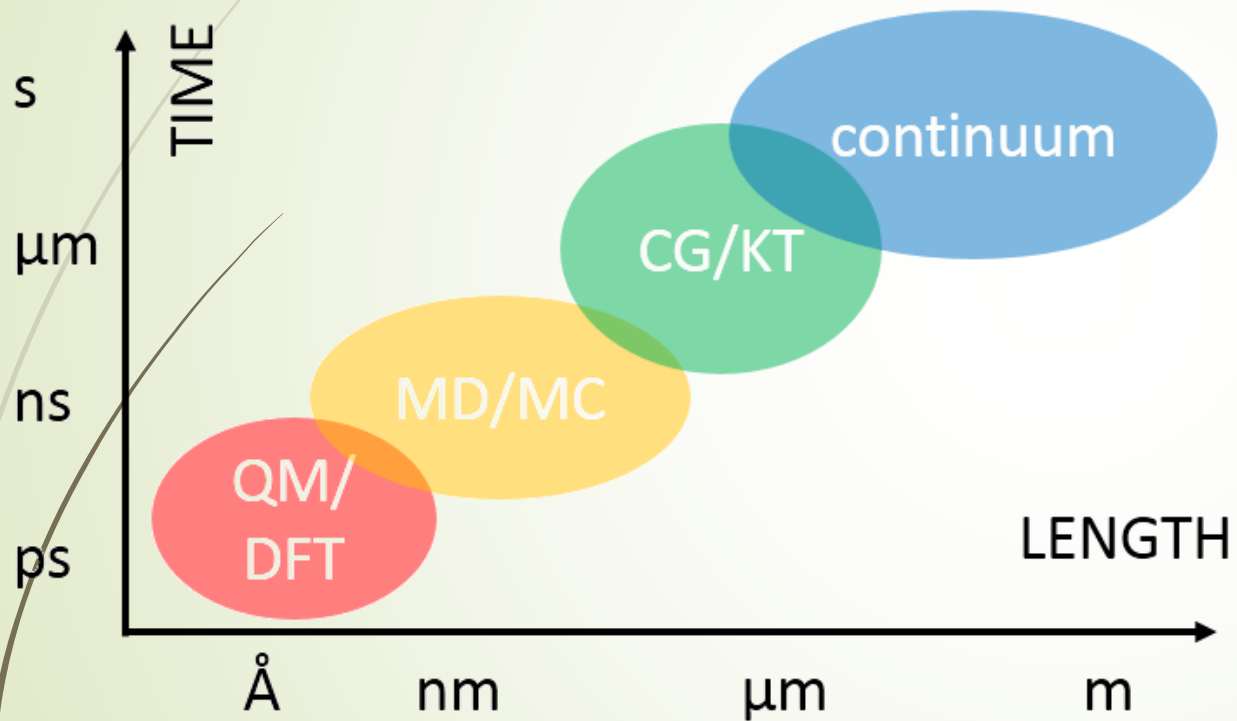
By: Bohayra Mortazavi

Email: [bohayra.mortazavi@iop.uni-hannover.de](mailto:bohayra.mortazavi@iop.uni-hannover.de) or [bohayra.mortazavi@gmail.com](mailto:bohayra.mortazavi@gmail.com)

Tel: +49 511 762 4126 or +49 157 8037 8770

# Multiscale modelling

## Why multiscale modelling?



DELTA GEN

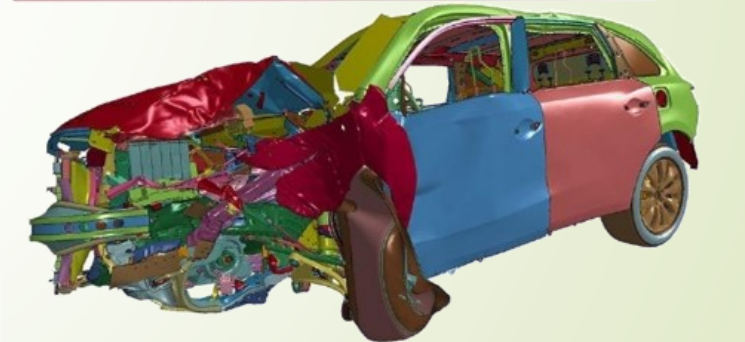
**HONDA**  
The Power of Dreams



To this...  
Honda R&D Americas, Inc. May 2014

Simulation Postprocessor

**HONDA**  
The Power of Dreams



In 6 months of working with 3DXCITE we realized a dream of going from this ...

Honda R&D Americas, Inc. May 2014

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## Content

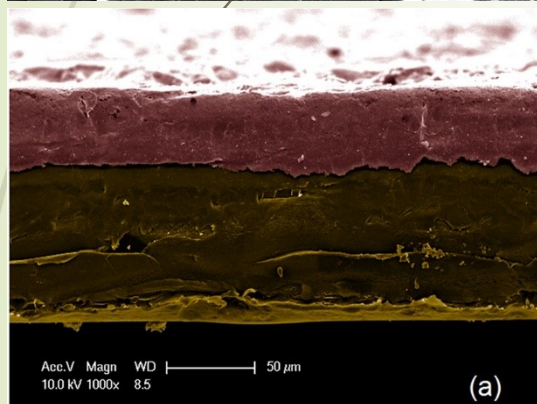
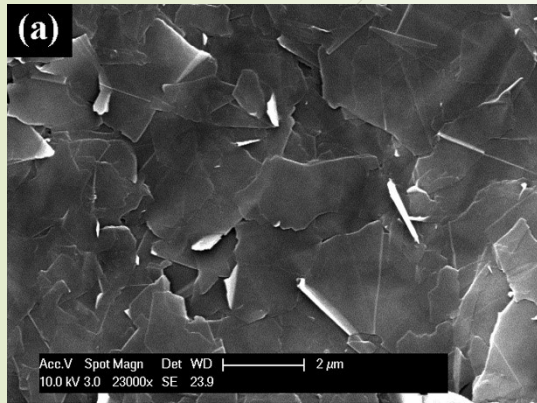
- **Empirical-based multiscale modeling.**
- Machine learning interatomic potentials and first-principles multiscale modeling.

# Empirical-based multiscale modeling

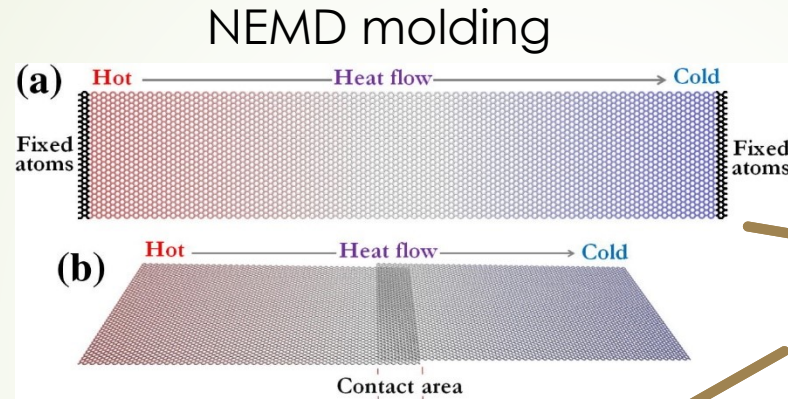
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## Example: Graphene or h-BN laminates:

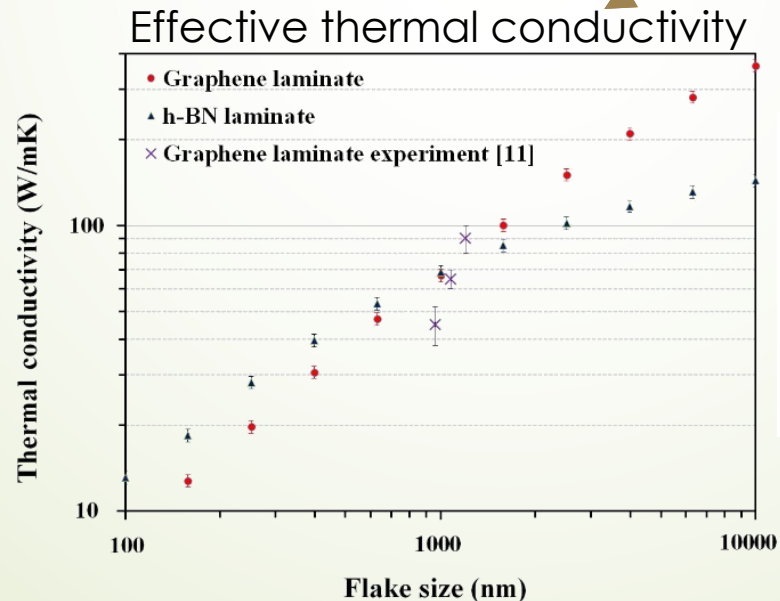
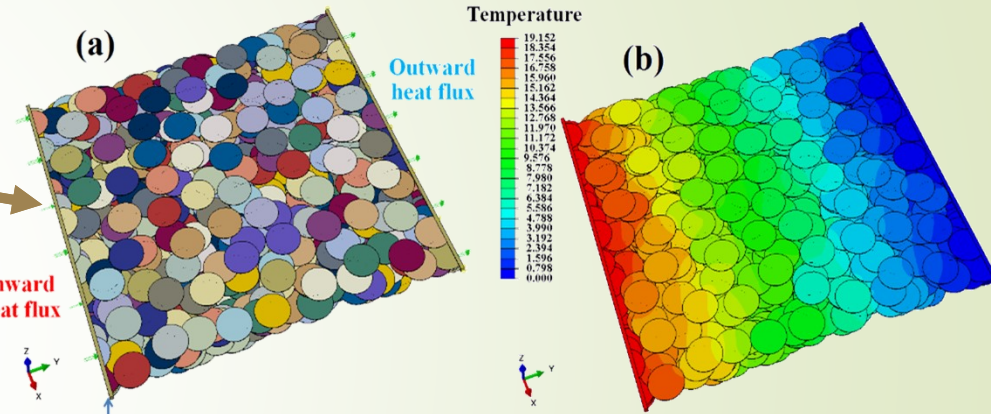
Experiments on graphene laminates



Nano Letters 14 (2014), 5155–5161



Finite element modeling



B Mortazavi and T Rabczuk. Carbon 85(2015), 1-7

IOP Publishing 2D Mater. 3 (2016) 011004 doi:10.1088/2053-1583/3/1/011004

**2D Materials**

LETTER

High thermal conductivity of hexagonal boron nitride laminates

Jin-Cheng Zheng<sup>1,2</sup>, Liang Zhang<sup>1</sup>, A V Kretinin<sup>3,4</sup>, S V Morozov<sup>4,5,6</sup>, Yi Bo Wang<sup>4</sup>, Tun Wang<sup>7</sup>, Xiaojun Li<sup>1</sup>, Fei Ren<sup>1</sup>, Jingyu Zhang<sup>8</sup>, Ching-Yu Lu<sup>8</sup>, Jia-Cing Chen<sup>8</sup>, Miao Lu<sup>7</sup>, Hui-Qiong Wang<sup>1,9</sup>, **A K Geim<sup>1</sup>** and **K S Novoselov<sup>4</sup>**

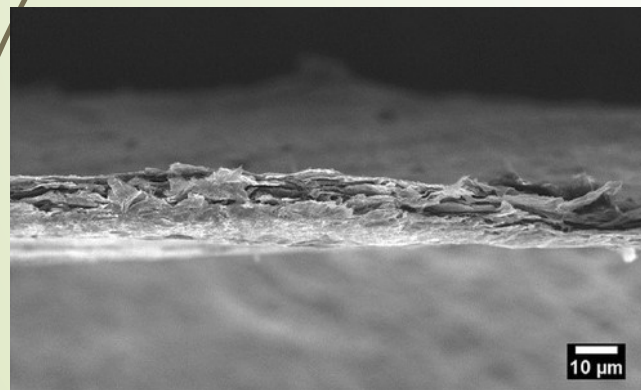
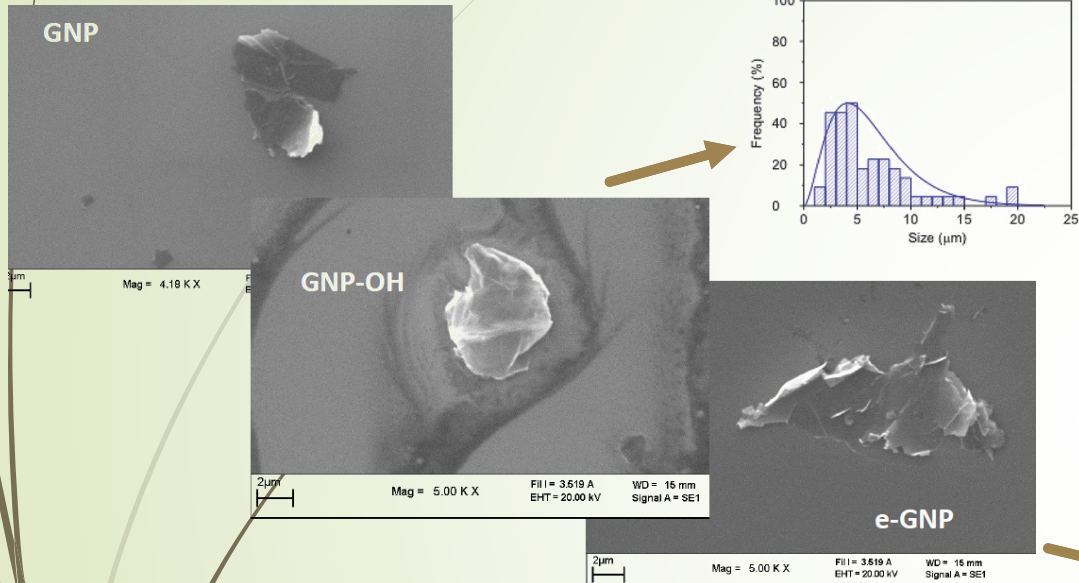
RECEIVED 17 November 2015  
 REVISED 10 December 2015  
 ACCEPTED FOR PUBLICATION 12 December 2015

# Empirical-based multiscale modeling

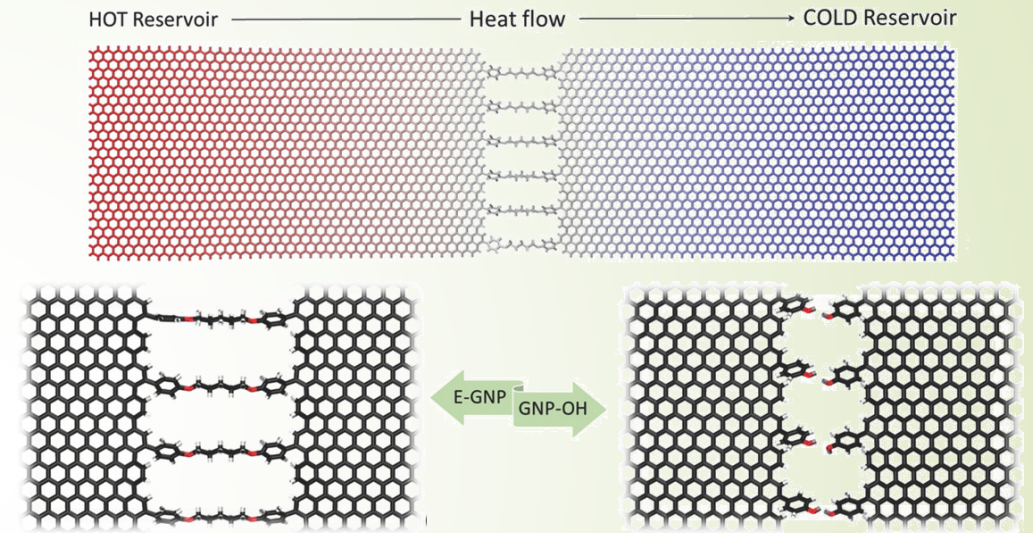
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## Example: Graphene laminates:

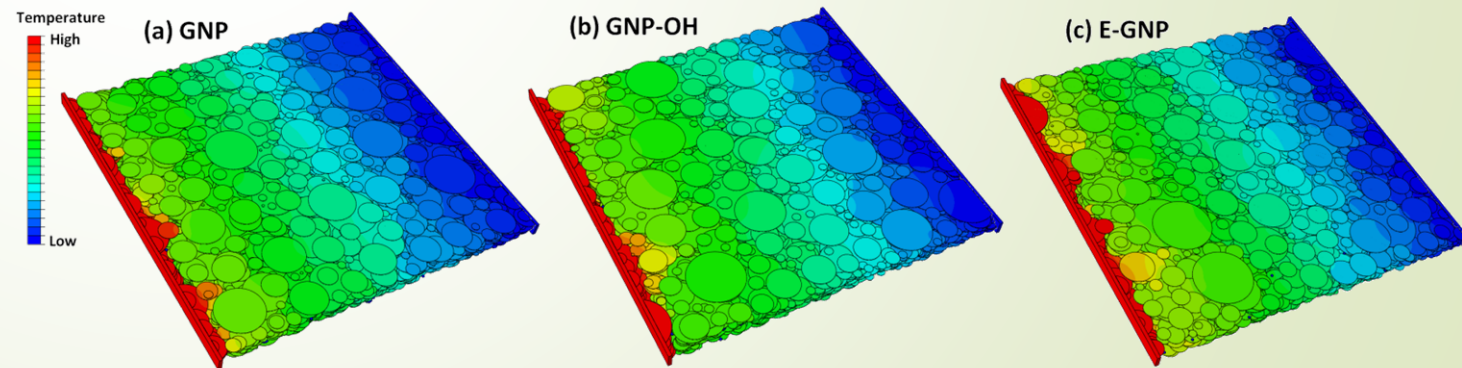
Experiment



MD modeling



Finite element modeling



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## Content

- ▶ Empirical-based multiscale modeling.
- ▶ **Machine learning interatomic potentials and first-principles multiscale modeling.**

# First-principles multiscale modeling

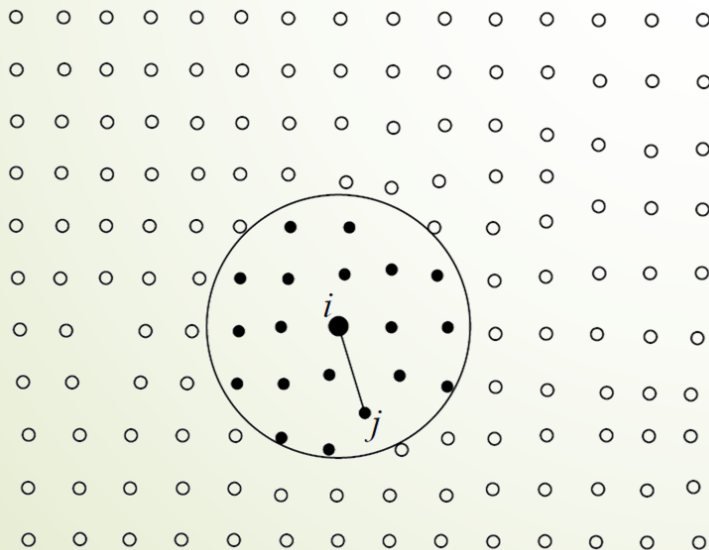
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## Concept:

- For the so-far presented studies, we were completely dependent on the empirical information and therefore for novel materials, compositions and structures the modeling becomes very restricted.
- Machine learning interatomic potentials (**MLIPs**) enable **first-principles multiscale modeling** and bridging the quantum mechanics to the continuum scale.

# Machine learning for defining atomic interactions

- ▶ Data-driven and multidimensional.
- ▶ Problem: Given  $E^{\text{qm}}(\mathbf{x})$ , interpolate it with a (machine-learning) model  $E(\mathbf{x})$  ( $\mathbf{x}$  is an atomic configuration)
- ▶ We want to minimize  $|E - E^{\text{qm}}|$ .
- ▶ We, Generate data:  $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots; E^{\text{qm}}(\mathbf{x}^{(1)}), E^{\text{qm}}(\mathbf{x}^{(2)}), \dots, \mathbf{f}^{\text{qm}}(\mathbf{x}^{(1)}), \dots$
- ▶ Minimize on data:  $\sum_i |E(\mathbf{x}^{(i)}) - E^{\text{qm}}(\mathbf{x}^{(i)})|^2 + (\text{forces}) + \dots$



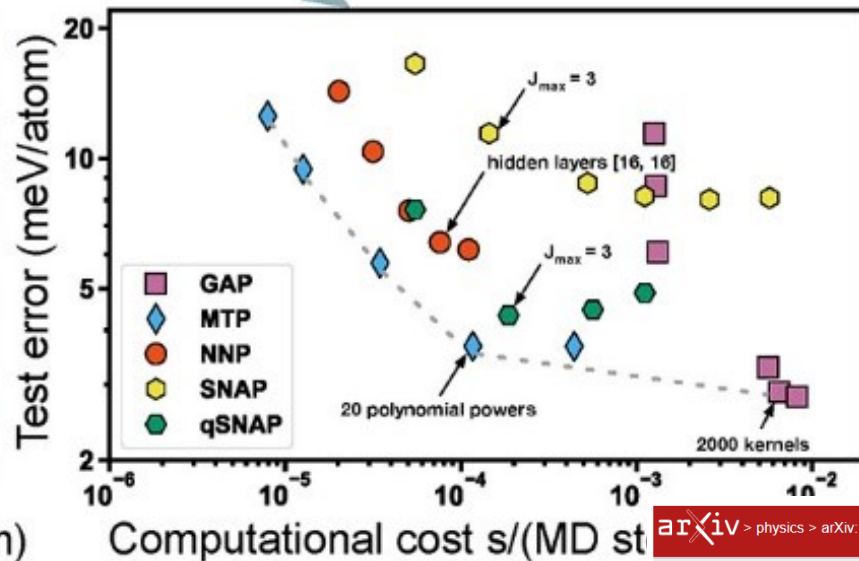


# Why Moment Tensor Potentials (MTPs)

## Machine Learning Interatomic Potentials

	Ni	Cu	Li	Mo	Si	Ge
GAP	0.62	0.60	0.75	3.01	4.49	4.02
MTP	0.66	0.52	0.73	3.53	3.24	4.46
NNP	2.38	2.13	1.24	6.06	10.84	11.27
SNAP	1.59	1.04	1.39	8.45	8.10	11.82
qSNAP	0.82	1.41	1.10	4.68	6.99	10.44
	1.04	1.16	0.85	3.96	6.28	10.55

RMSE energy error (meV/atom)



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**Alexander Shapeev**

Associate Professor  
Center for Energy Science and Technology

I have graduated from Novosibirsk State University in 2001 with Bachelor degree and in 2003 with Master degree. I got my PhD from National University of Singapore in 2009 on this topic of computational fluid mechanics.

J. Phys. Chem. A 2020, 124, 4, 731–745

arXiv > physics > arXiv:1906.08888

Physics > Computational Physics

[Submitted on 20 Jun 2019 (v1), last revised 24 Jul 2019 (this version, v4)]

**A Performance and Cost Assessment of Machine Learning Interatomic Potentials**

Yunxing Zuo, Chi Chen, Xiangguo Li, Zhi Deng, Yiming Chen, Jörg Behler, Gábor Csányi, Alexander V. Shapeev, Aidan P. Thompson, Mitchell A. Wood, Shyue Ping Ong

Machine learning of the quantitative relationship between local environment descriptors and the potential energy surface of a system of atoms has emerged as a new frontier in the development of functions, smooth overlap of atomic positions (SOAP), the Spectral Neighbor Analysis Potential (SNAP) bispectrum components, and moment tensors --- using a diverse data set generated using (Si, Ge) is chosen to span a range of crystal structures and bonding. All descriptors studied show excellent performance in predicting energies and forces far surpassing that of classical IAPs, as freedom of each model, and consequently computational cost. We will discuss these trade-offs in the context of model selection for molecular dynamics and other applications.

# First-principles multiscale modeling

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## Thermal transport

SCIENCE ADVANCES | RESEARCH ARTICLE

MATERIALS SCIENCE

### Borophene-graphene heterostructures

Xiaolong Liu<sup>1</sup> and Mark C. Hersam<sup>1,2,3,4\*</sup>

Integration of dissimilar two-dimensional (2D) materials is essential for nanoelectronic applications. Compared to vertical stacking, covalent lateral stitching requires bottom-up synthesis, resulting in rare realizations of 2D lateral heterostructures. Because of its polymorphism and diverse bonding geometries, borophene is a promising candidate for 2D heterostructures, although suitable synthesis conditions have not yet been demonstrated. Here, we report lateral and vertical integration of borophene with graphene. Topographic and spatially resolved spectroscopic measurements reveal nearly atomically sharp lateral interfaces despite imperfect crystallographic lattice and symmetry matching. In addition, boron intercalation under graphene results in rotationally commensurate vertical heterostructures. The rich bonding configurations of boron suggest that borophene can be integrated into a diverse range of 2D heterostructures.

Computationally not feasible



Not accurate and/or stable

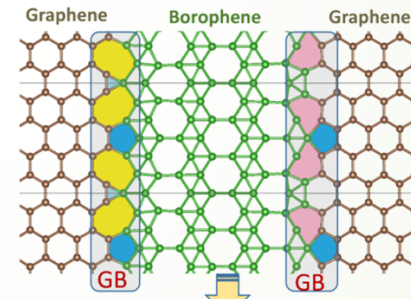


Solution



### Key steps:

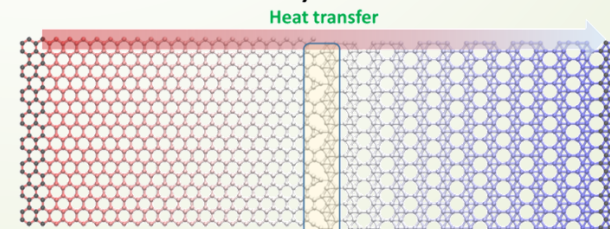
#### 1. Ab-initio molecular dynamics simulations



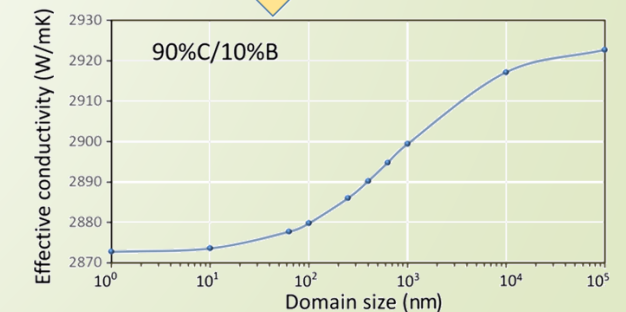
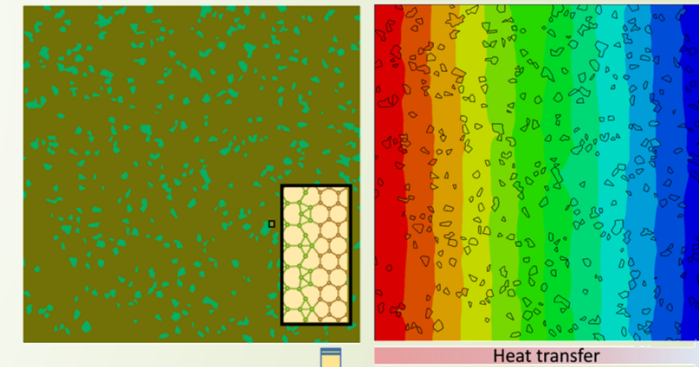
#### 2. Machine-learning interatomic potentials

Moment tensor potentials (MTPs):  $v(\mathbf{r}_i) = \sum_{j=1}^m \theta_j B_j(\mathbf{r}_i)$ .

#### 3. Classical molecular dynamics simulations



#### 4. Finite element modeling of graphene/borophene heterostructures



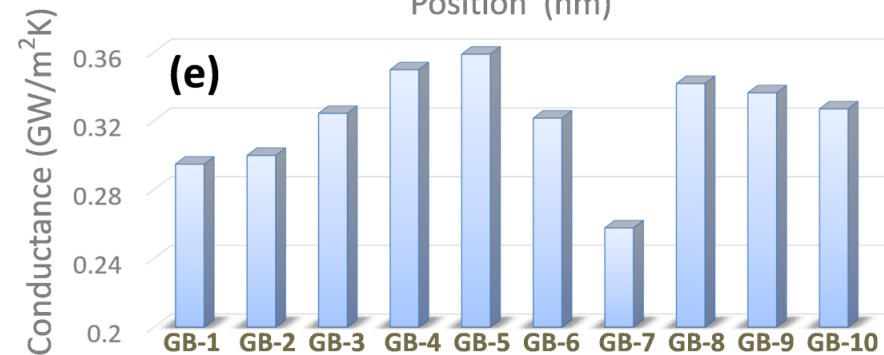
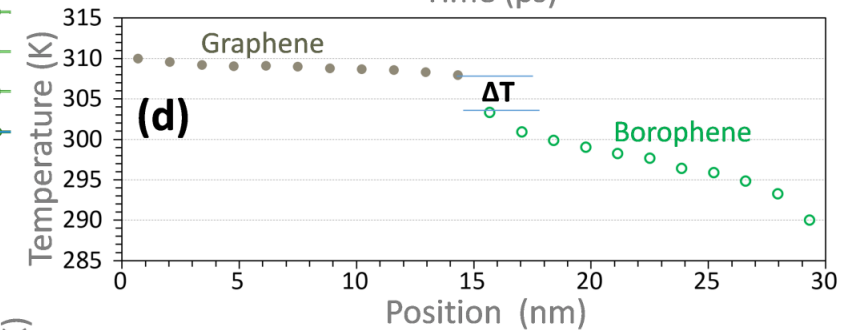
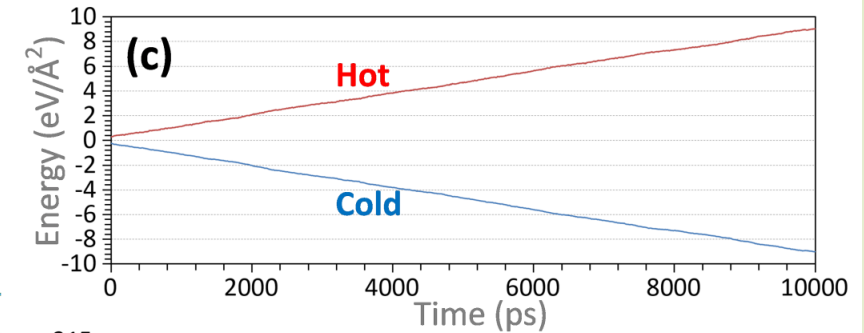
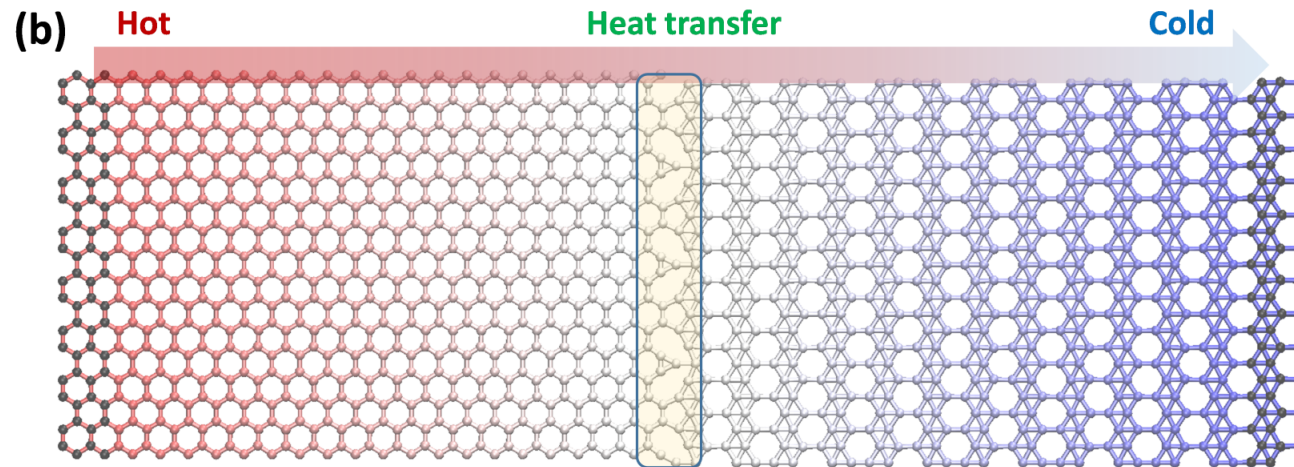
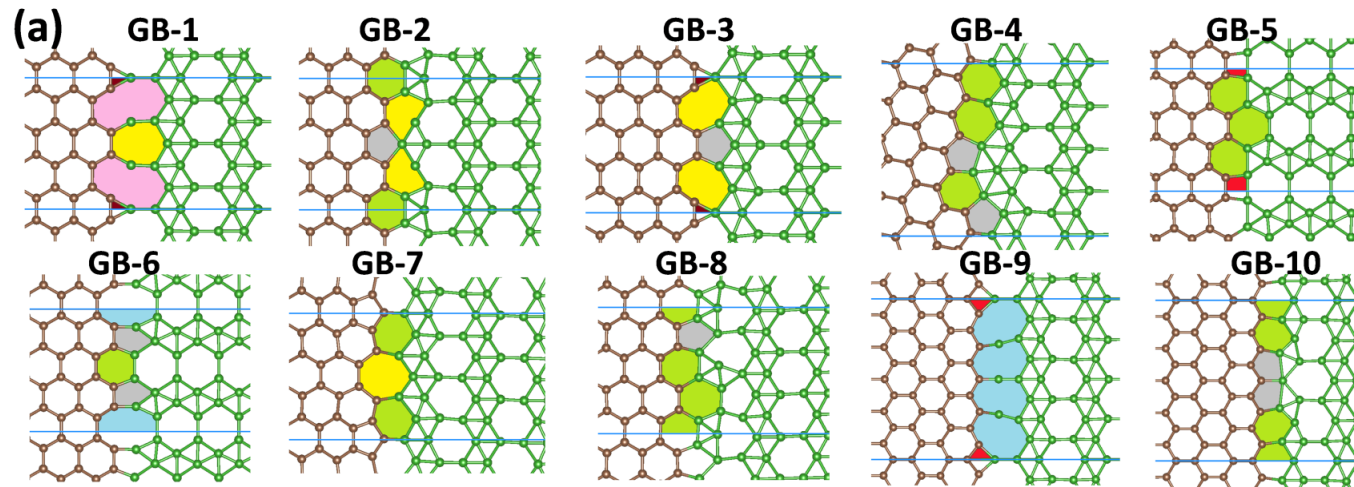
# First-principles multiscale modeling

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## Thermal transport

Machine Learning Interatomic Potentials Enable First-Principles Multiscale Modeling of Lattice Thermal Conductivity in Graphene/Borophene Heterostructures

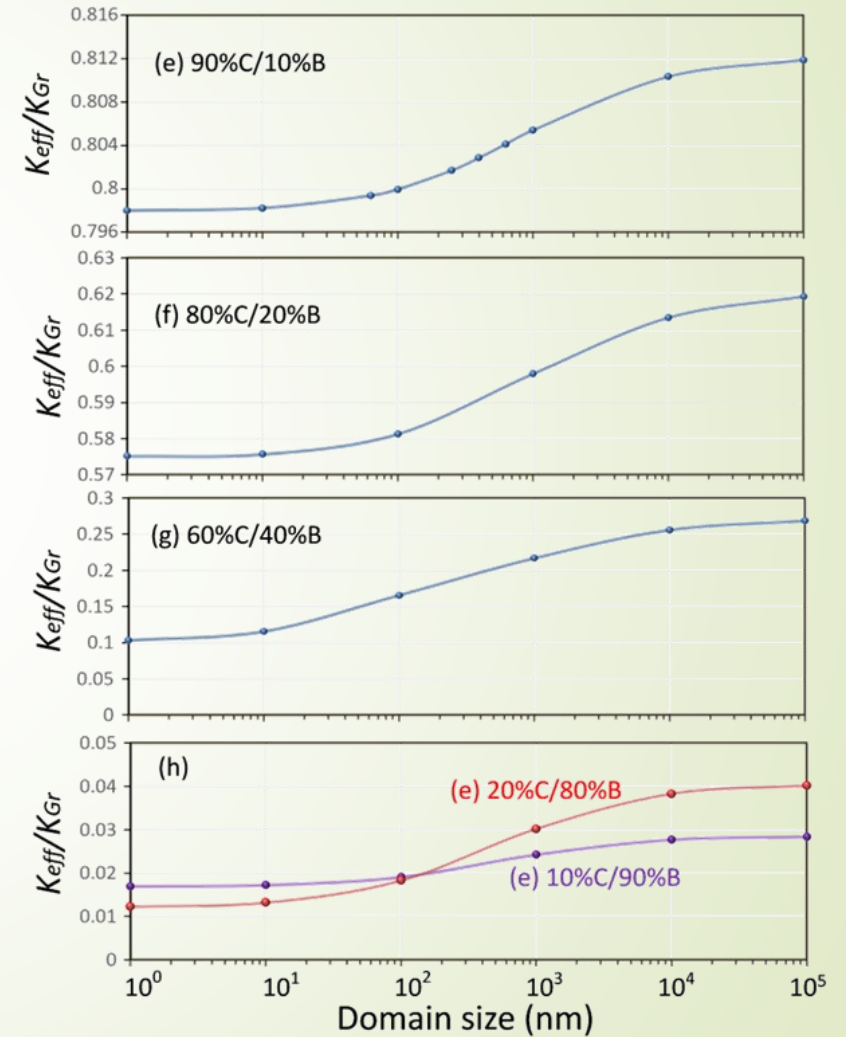
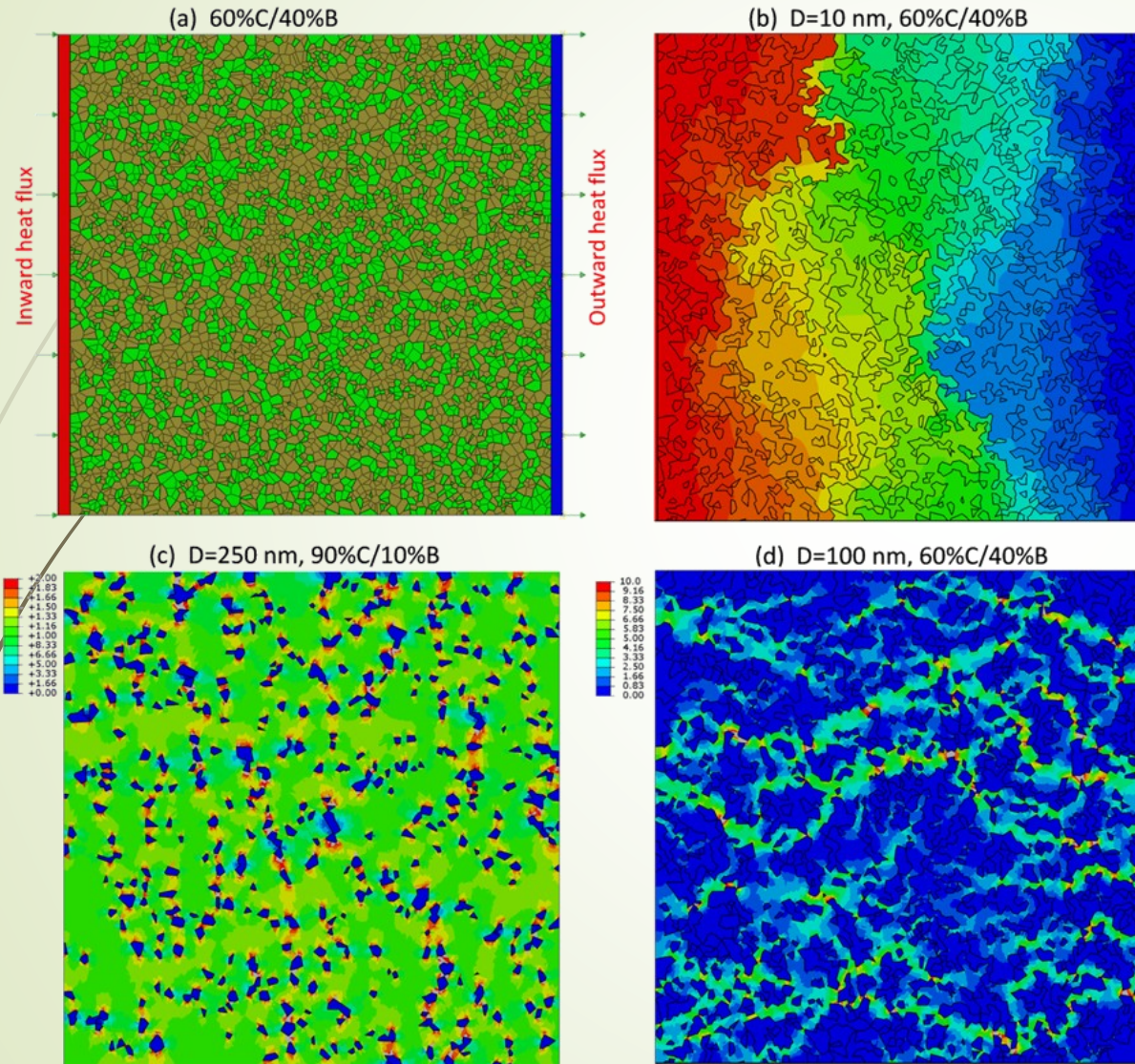
<http://dx.doi.org/10.17632/pbgscy3ptg.1>



# First-principles multiscale modeling

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## Thermal transport

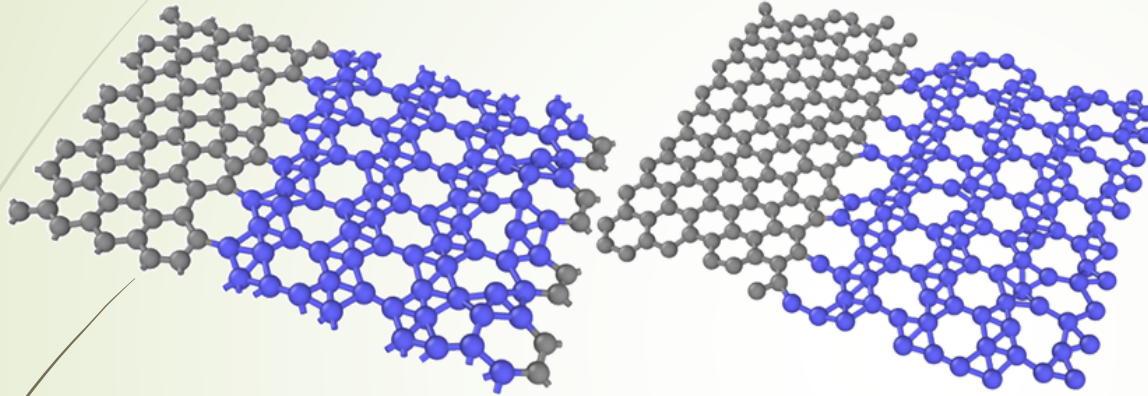


# First-principles multiscale modeling

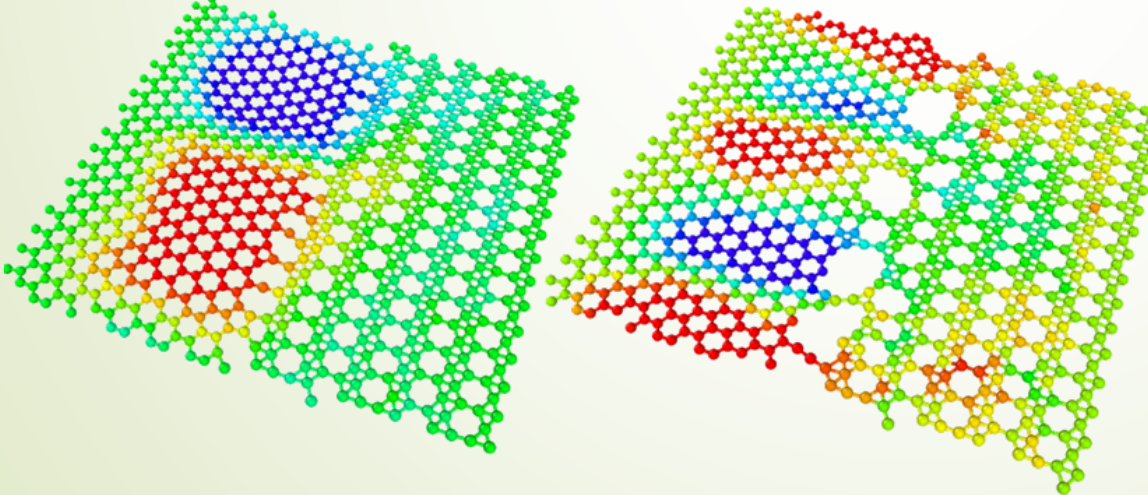
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## Mechanical properties

**Step 1: Ab-initio calculations and dataset creation**



**Step 3: Classical molecular dynamics simulations**



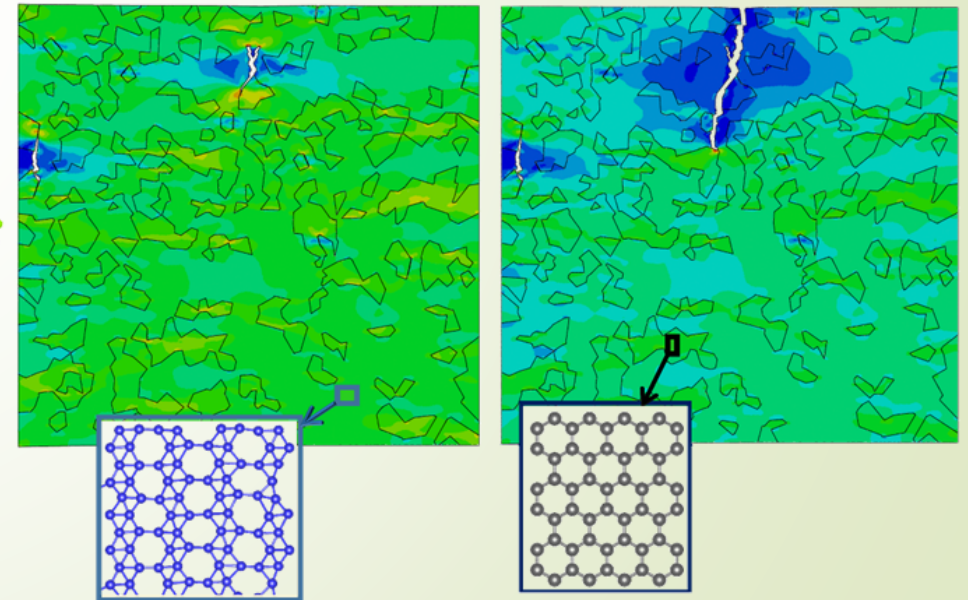
**Step 2: Machine-learning interatomic potentials**

**Moment tensor potentials (MTPs):**

$$V(\mathbf{n}_i) = \sum_{\alpha} \xi_{\alpha} B_{\alpha}(\mathbf{n}_i),$$

$$M_{\mu,\nu}(\mathbf{n}_i) = \sum_j f_{\mu}(|r_{ij}|, z_i, z_j) r_{ij} \otimes \dots \otimes r_{ij},$$

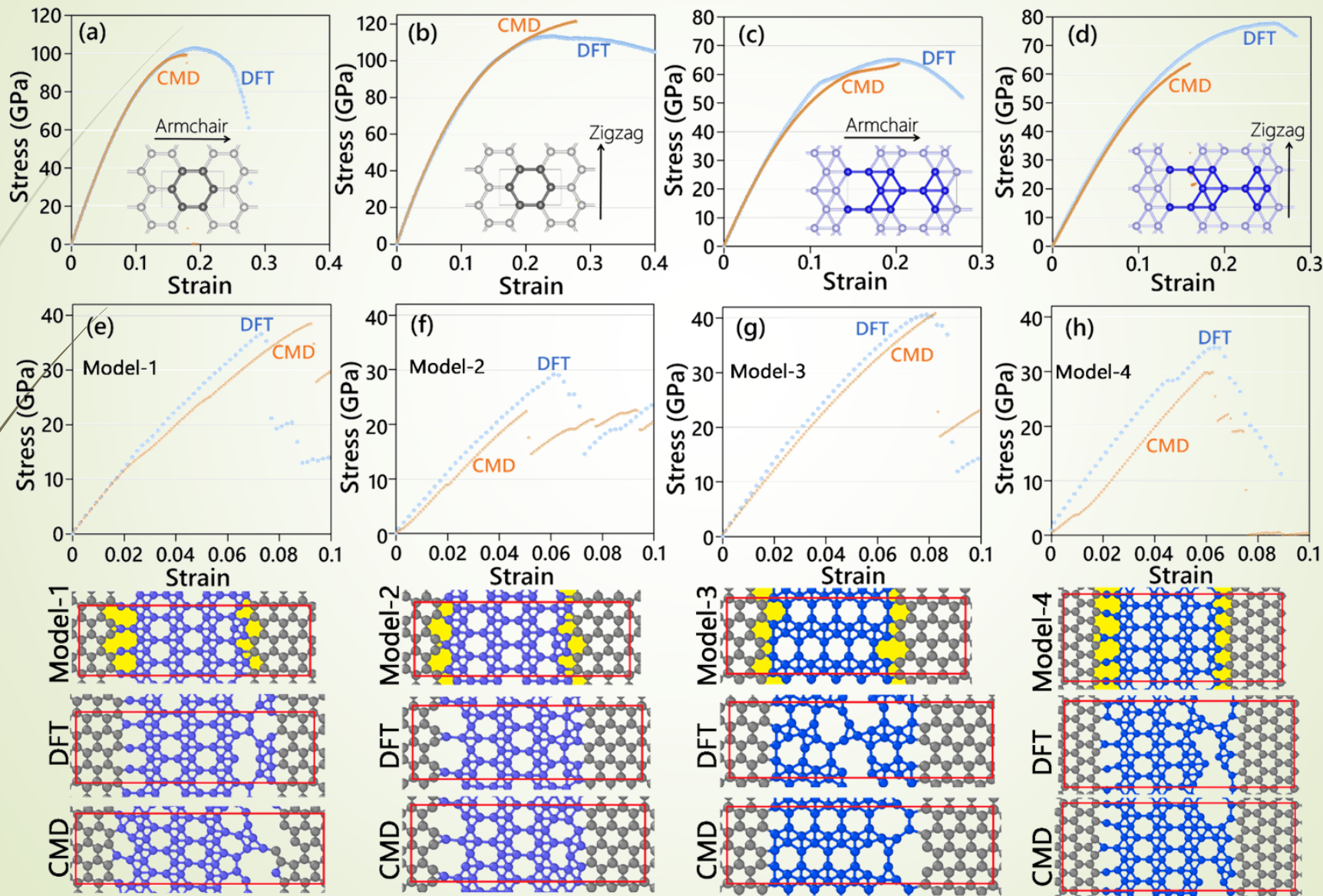
**Step 4: Continuum finite element modeling**



# First-principles multiscale modeling

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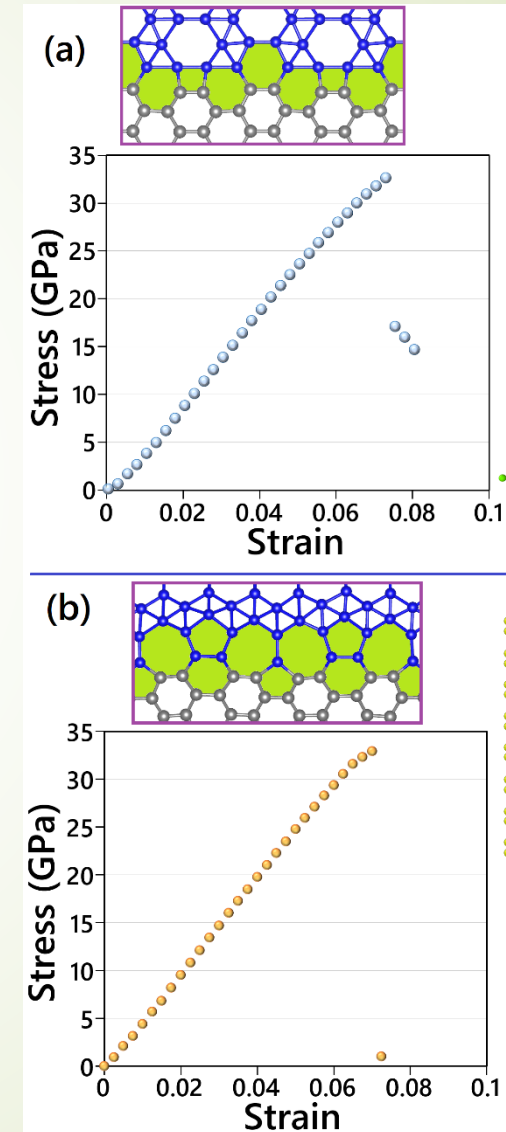
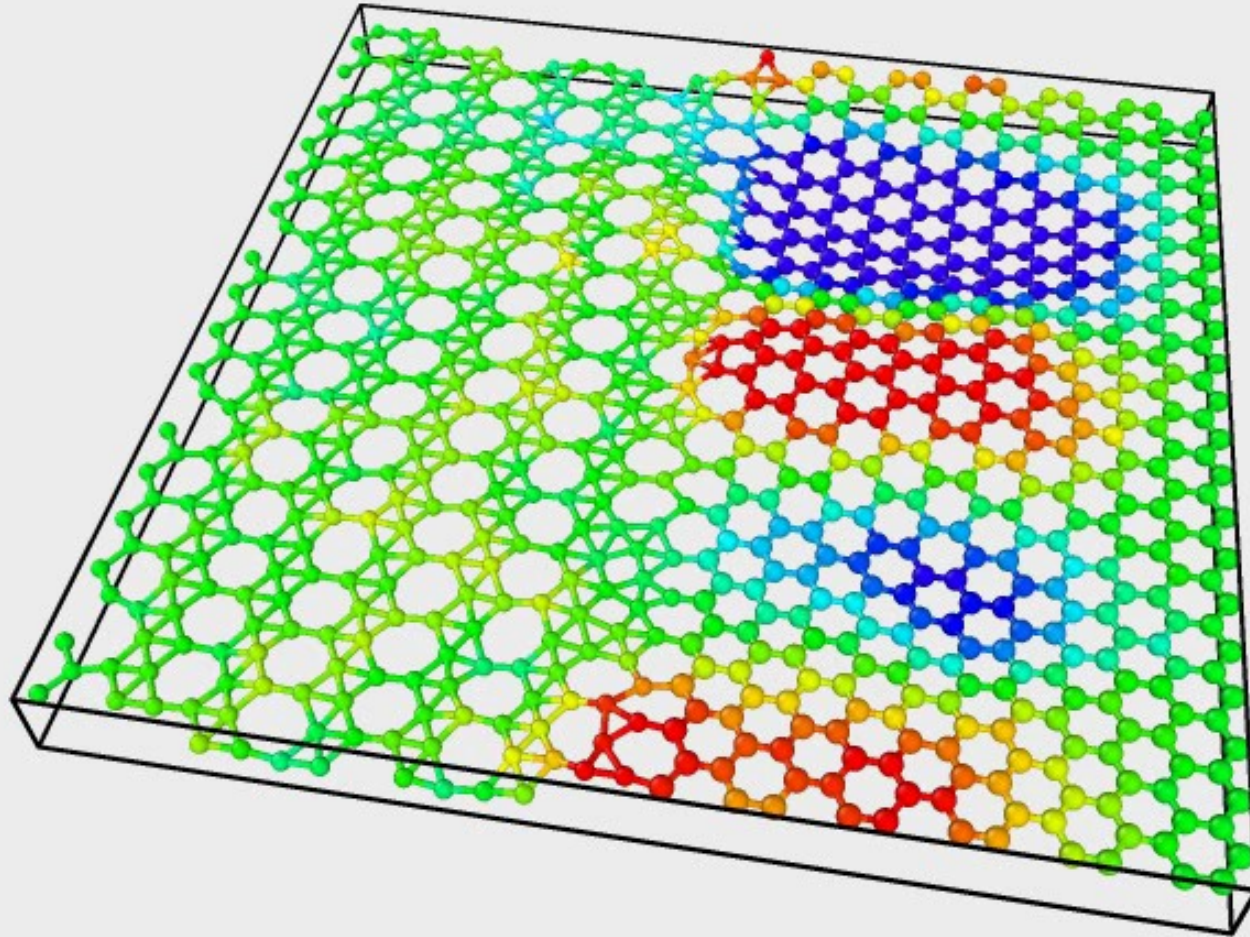
## Mechanical properties



# First-principles multiscale modeling

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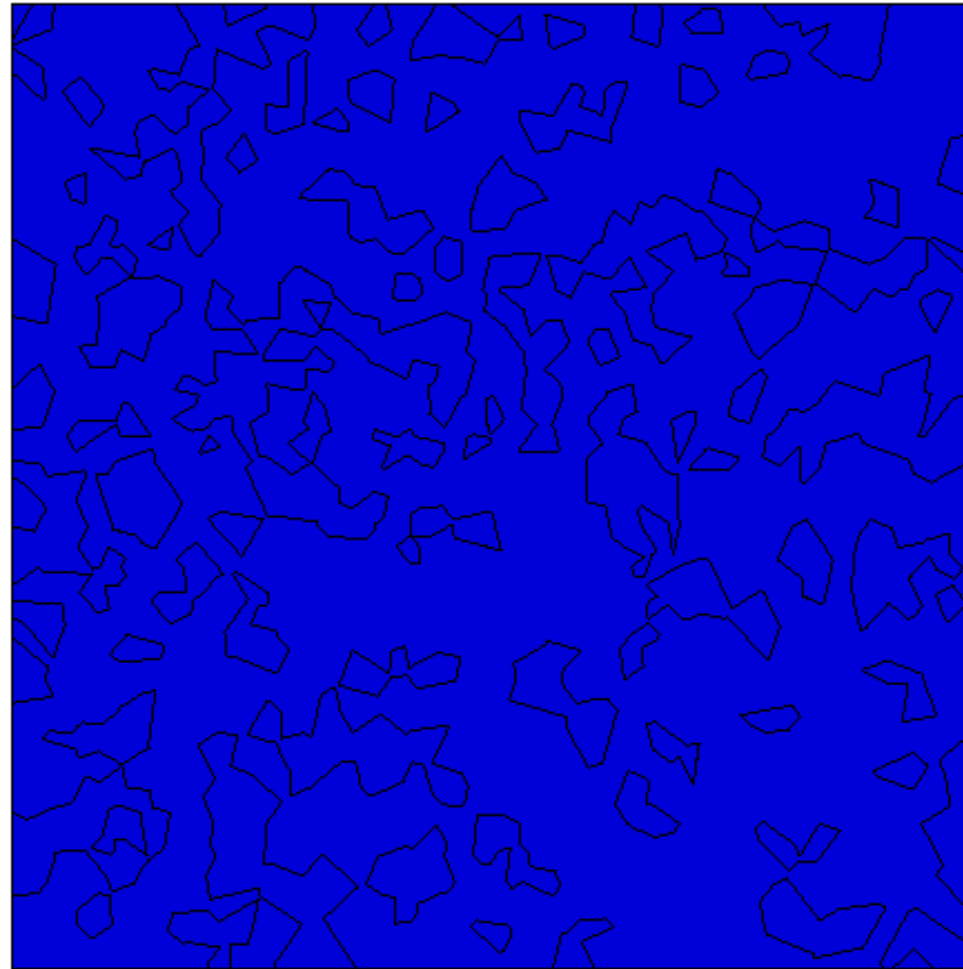
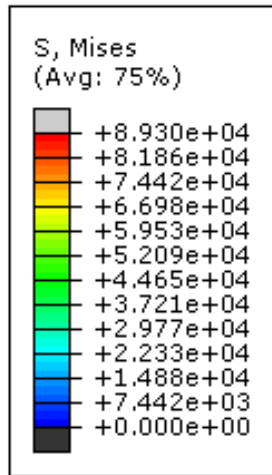
## Mechanical properties



# First-principles multiscale modeling

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## Mechanical properties



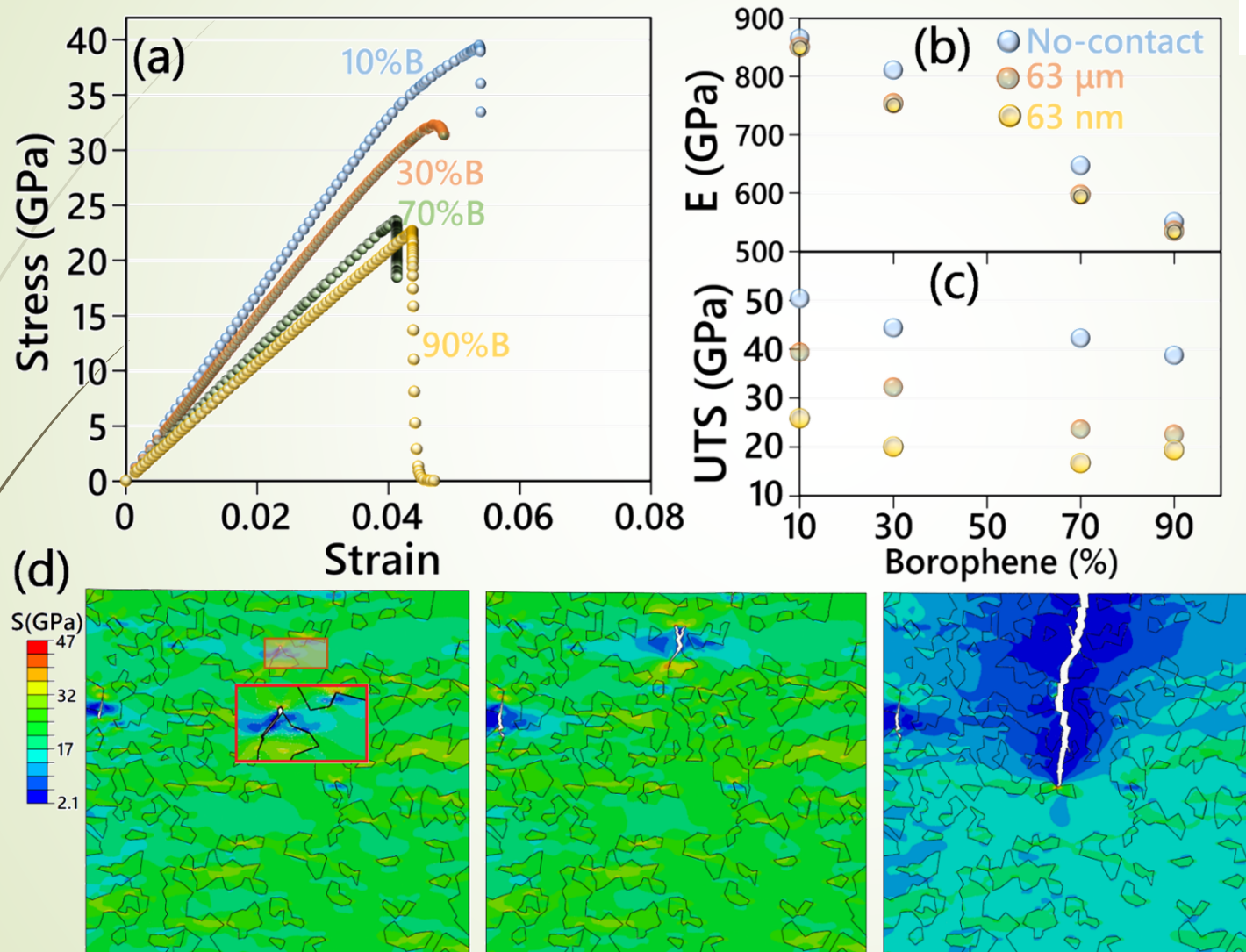
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# First-principles multiscale modeling

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## Mechanical properties



Mendeley Data

First-Principles Multiscale Modeling of Mechanical Properties in Graphene/Borophene Heterostructures Empowered by Machine-Learning Interatomic Potentials

Published: 11 May 2021 | Version 1 | DOI: 10.17632/yrm7p7w37f.1  
Contributor: Bohayra Mortazavi

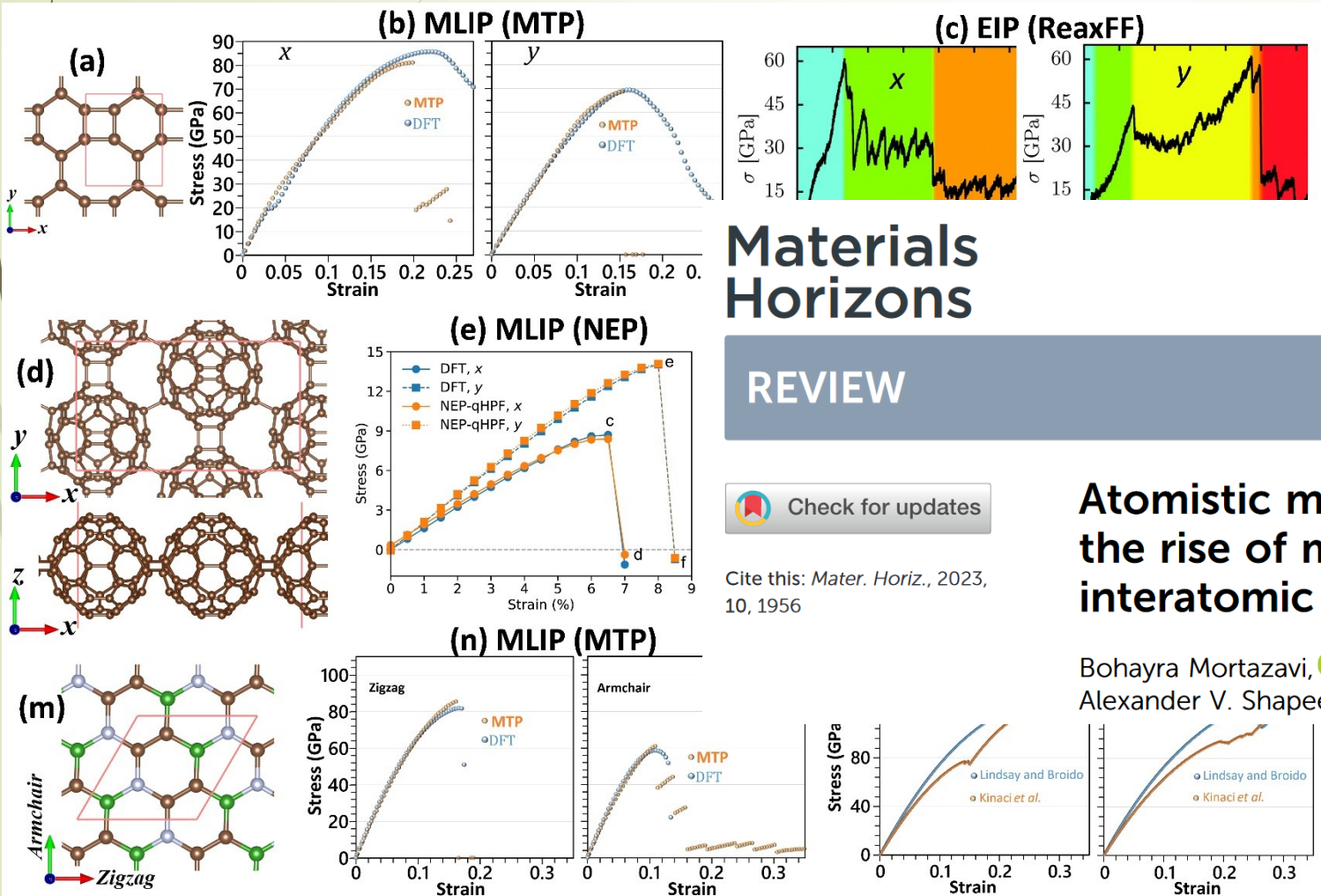
<http://dx.doi.org/10.17632/pbgscy3ptg.1>

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## Misguiding of empirical interatomic potentials

Considering novel 2D systems



Materials Horizons

REVIEW



Cite this: *Mater. Horiz.*, 2023, 10, 1956



Atomistic modeling of the mechanical properties: the rise of machine learning interatomic potentials

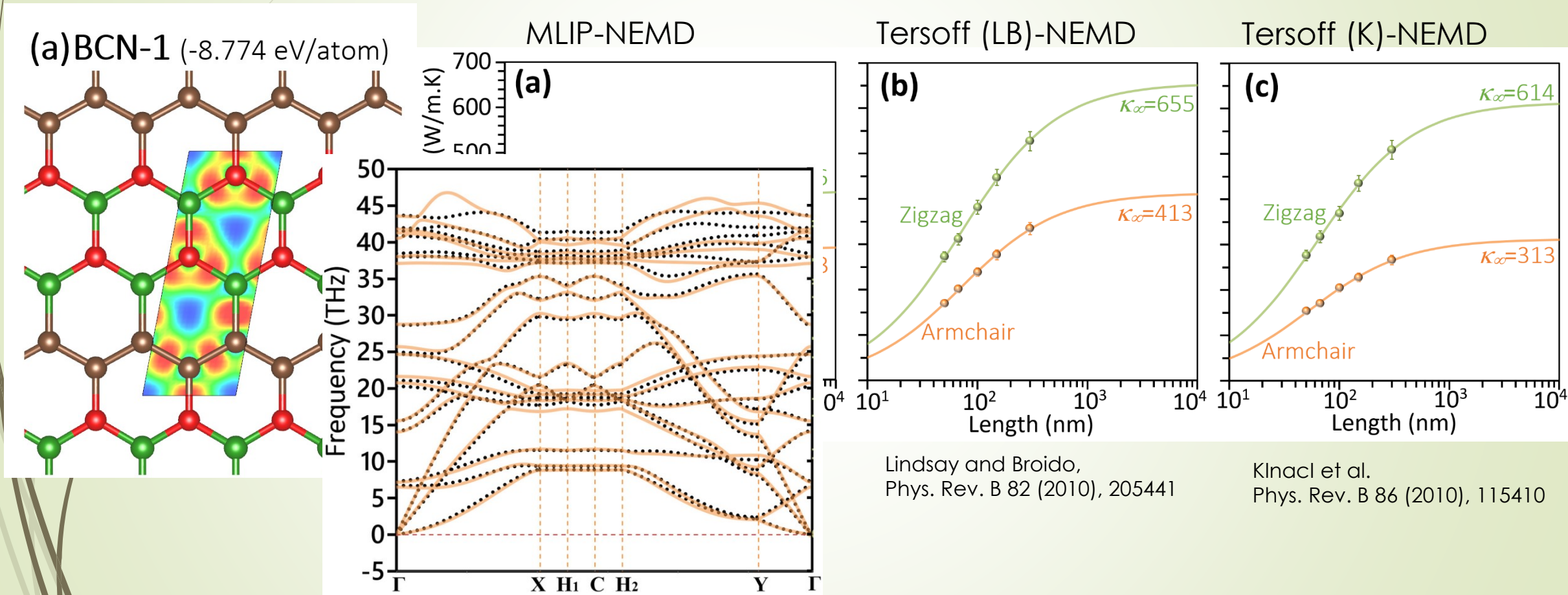
Bohayra Mortazavi,<sup>1</sup> Xiaoying Zhuang,<sup>2,3</sup> Timon Rabczuk<sup>4</sup> and Alexander V. Shapeev<sup>5</sup>

# First-principles multiscale modeling

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## Misguiding of empirical interatomic potentials

Comparison with empirical interatomic potentials



Lindsay and Broido,  
Phys. Rev. B 82 (2010), 205441

Klناcl et al.  
Phys. Rev. B 86 (2010), 115410

THANKS A LOT  
FOR YOUR  
ATTENTIONS  
QUESTIONS?