In the name of God

PhoenixD

Photonics · Optics · Engineering
Innovation Across Disciplines

Leibniz Universität Hannover

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

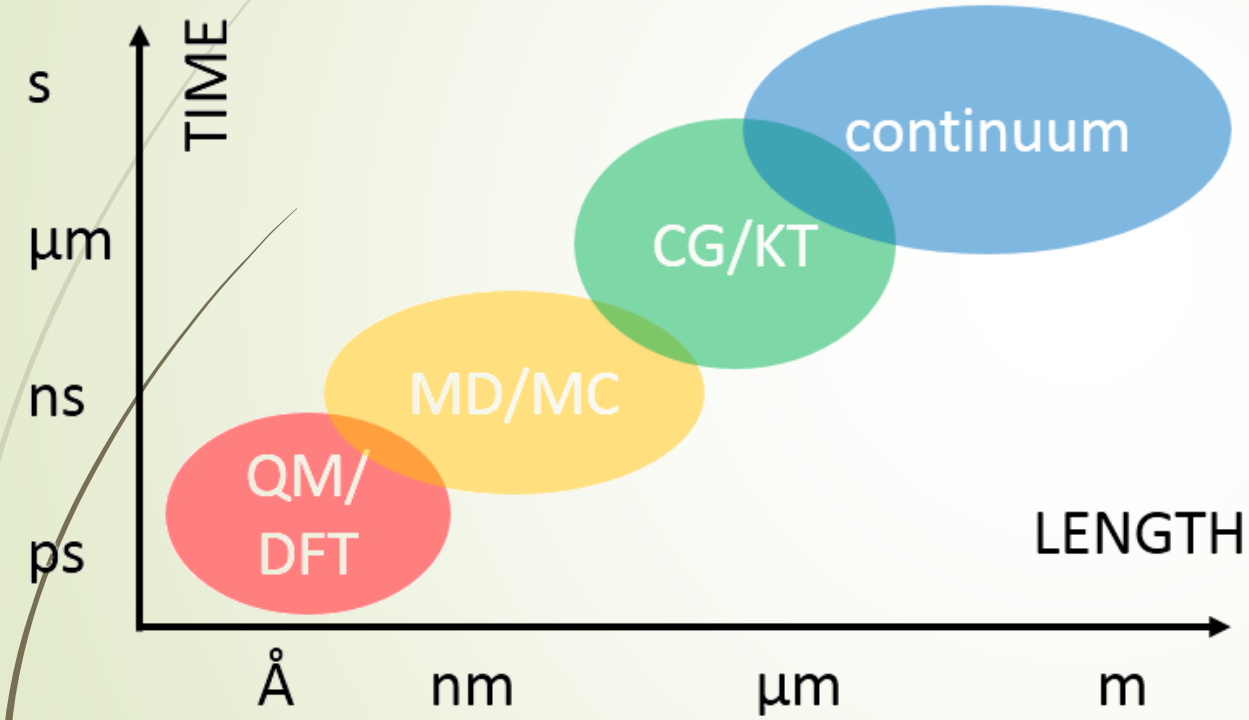
By: Bohayra Mortazavi

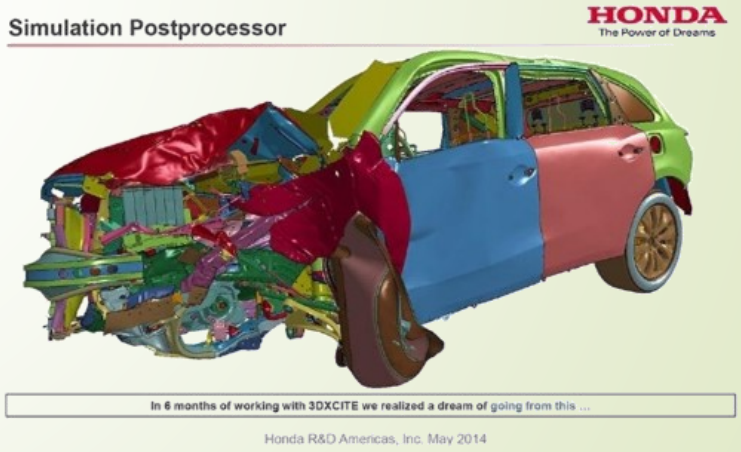
Email: bohayra.mortazavi@iop.uni-hannover.de or bohayra.mortazavi@gmail.com

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

Multiscale modelling

Why multiscale modelling?





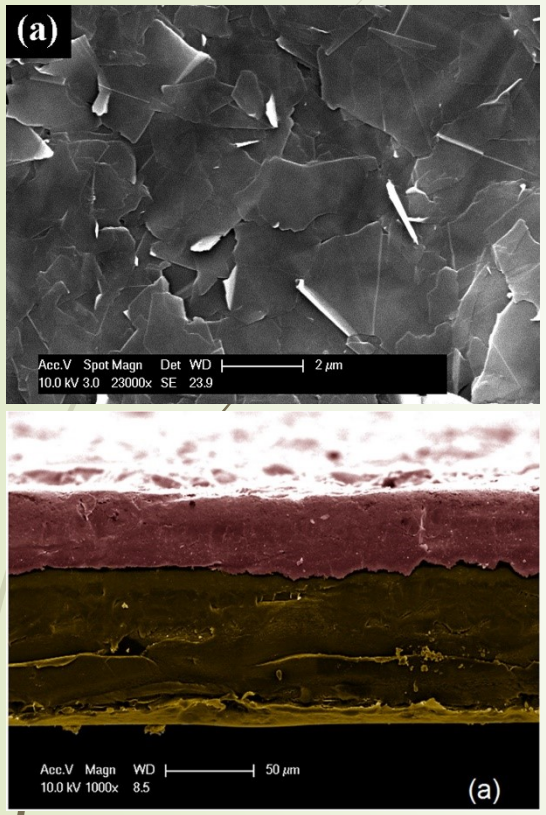
Content

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

Empirical-based multiscale modeling

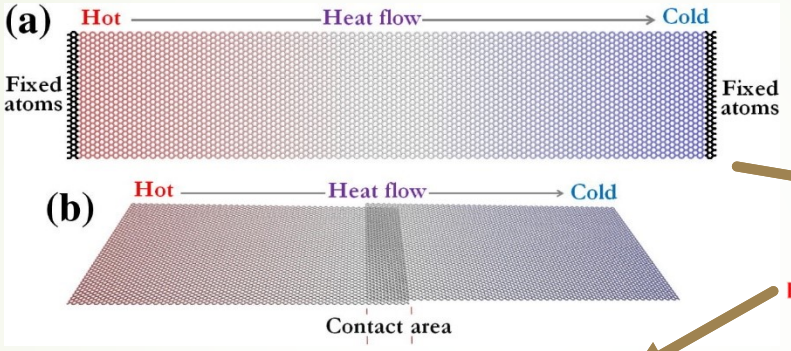
4 Example: Graphene or h-BN laminates:

Experiments on graphene laminates

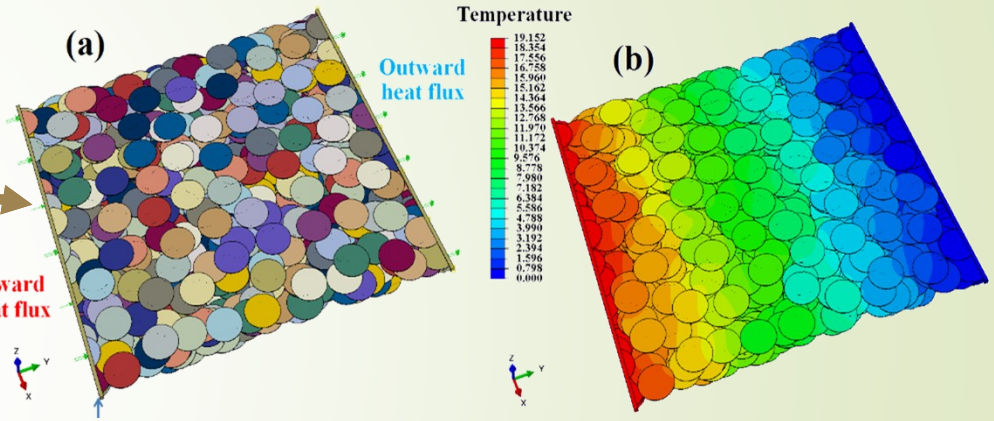


Nano Letters 14 (2014), 5155–5161

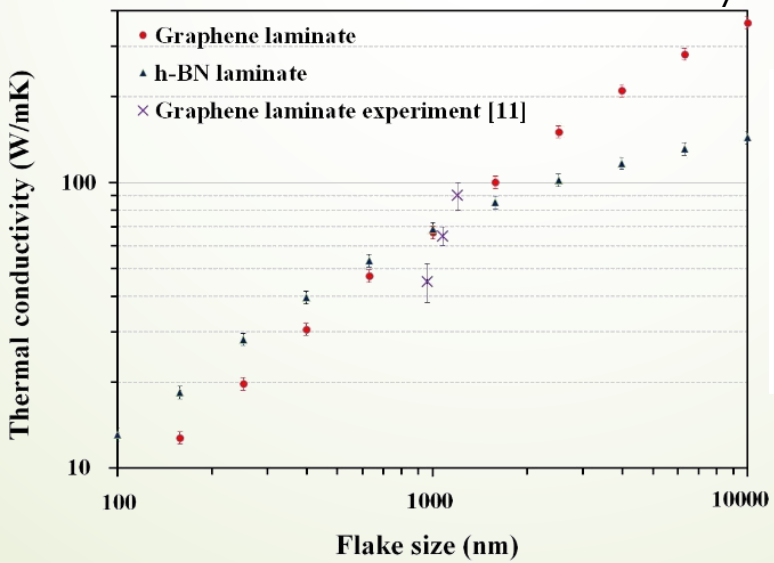
NEMD molding

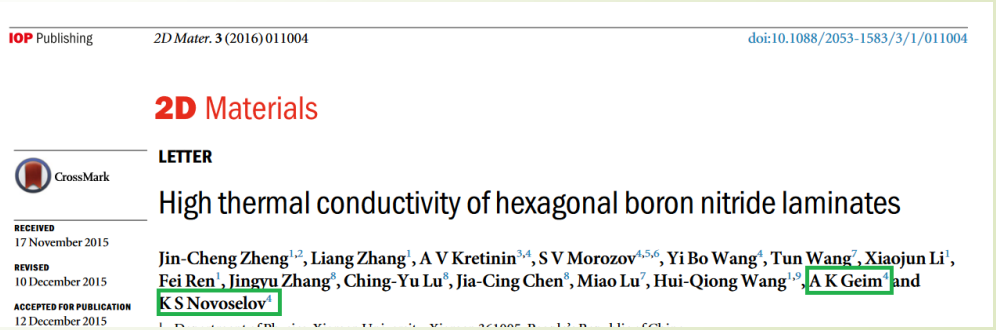


Finite element modeling



Effective thermal conductivity




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

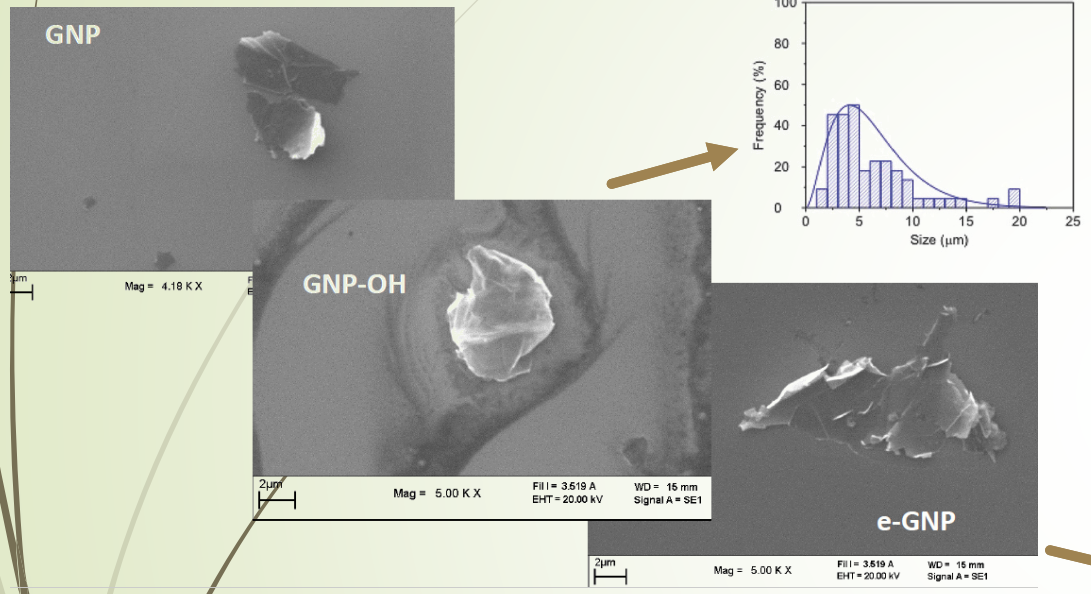
RECEIVED 17 November 2015
REVISED 10 December 2015
ACCEPTED FOR PUBLICATION 12 December 2015

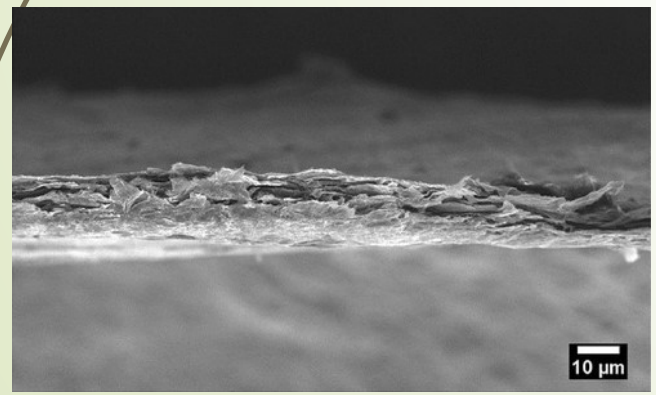
B Mortazavi and T Rabczuk. Carbon 85(2015), 1-7

Empirical-based multiscale modeling

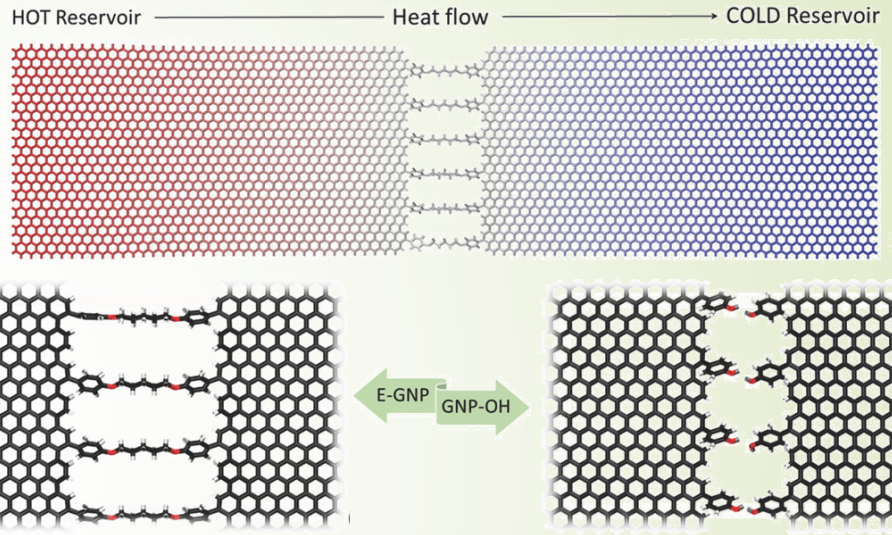
Example: Graphene laminates:

Experiment

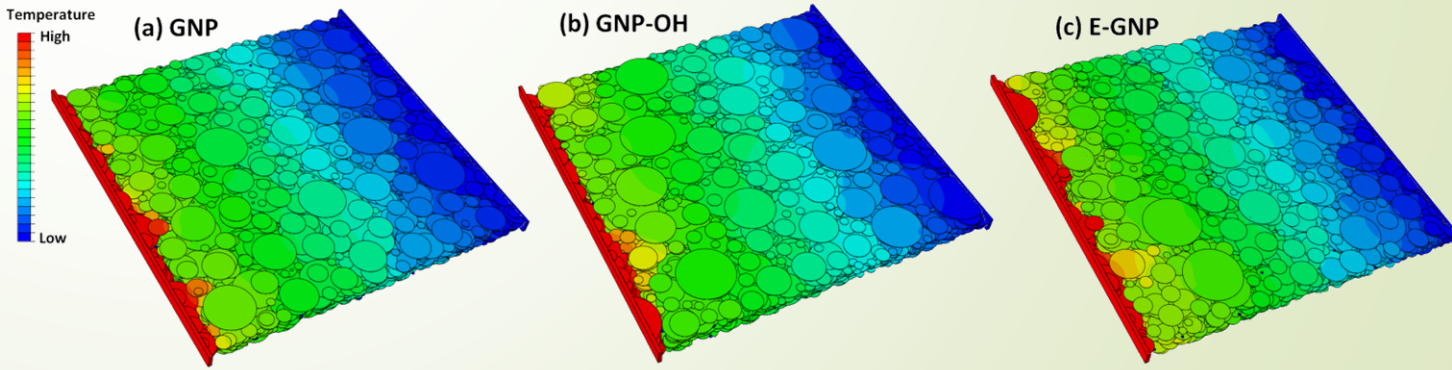




MD modeling



Finite element modeling



Advanced Functional Materials 28 (2018), 1706954

Content

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

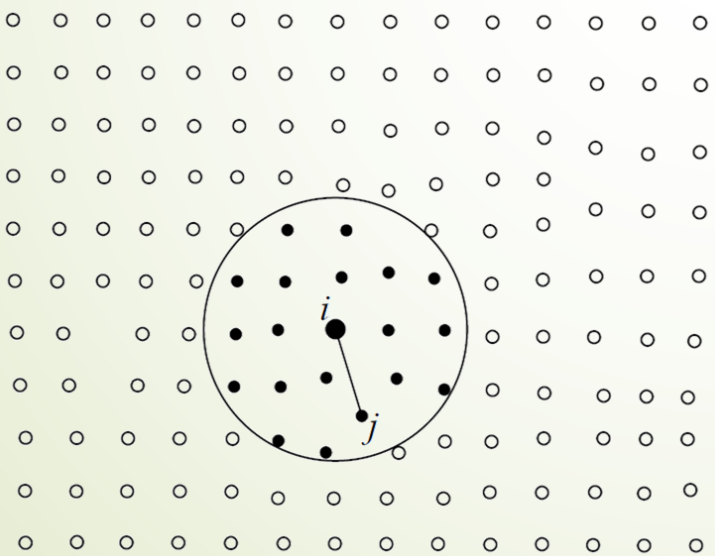
First-principles multiscale modeling

Concept:

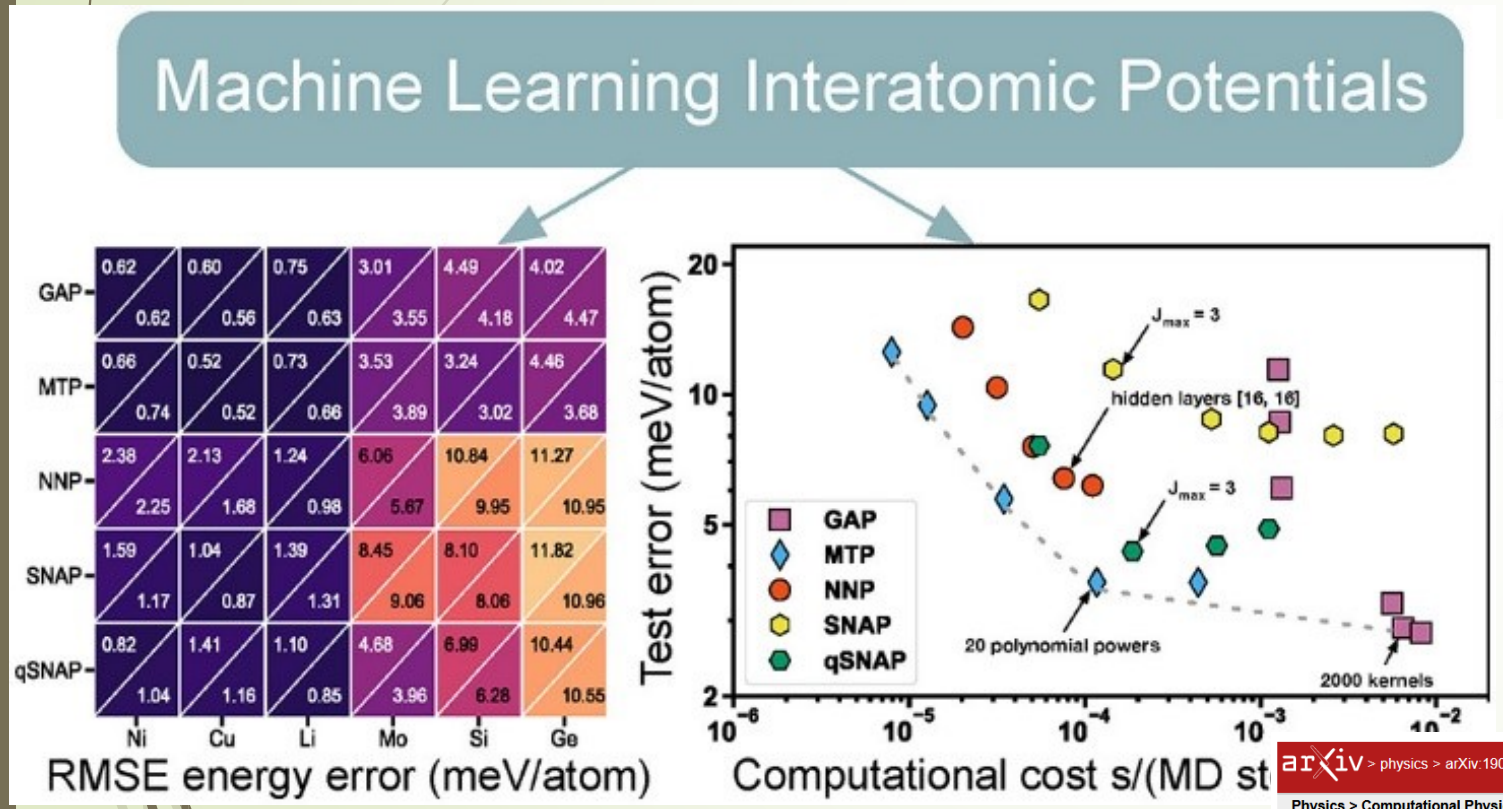
- For the so-far presented studies, we were completely dependent on the empirical information and therefore for novel materials, compositions and structures the modeling becomes very restricted.
- Machine learning interatomic potentials (**MLIPs**) enable **first-principles multiscale modeling** and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

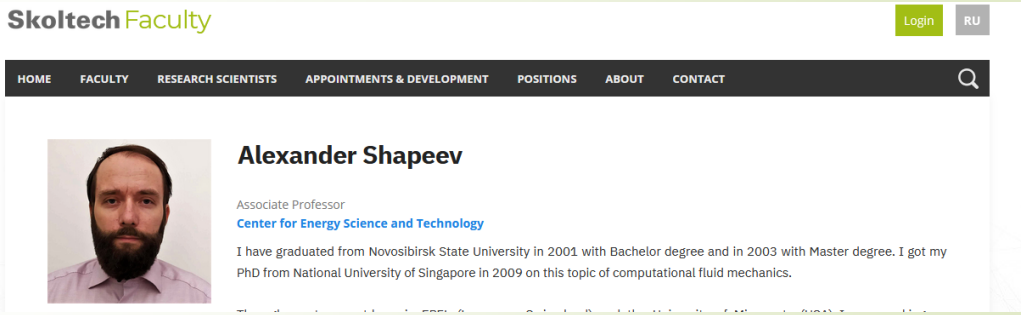
Machine learning for defining atomic interactions

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

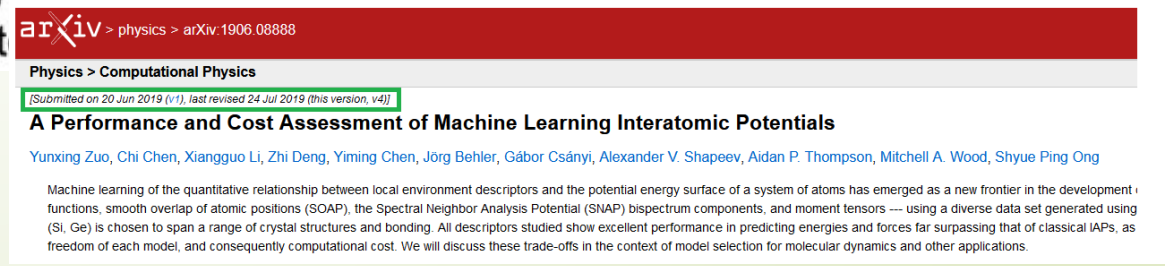


Why Moment Tensor Potentials (MTPs)





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



First-principles multiscale modeling

10

Thermal transport

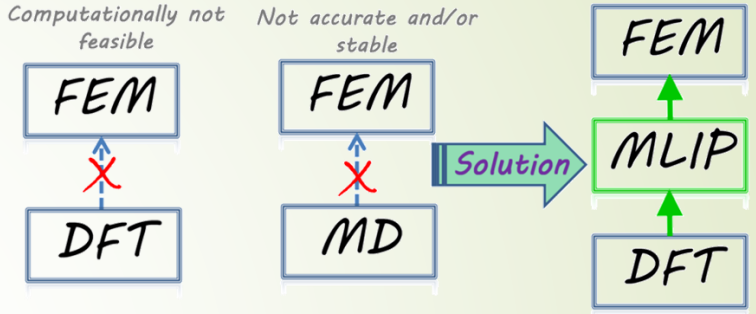
SCIENCE ADVANCES | RESEARCH ARTICLE

MATERIALS SCIENCE

Borophene-graphene heterostructures

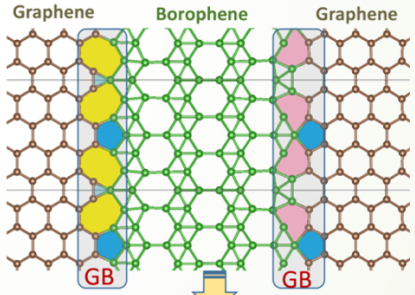
Xiaolong Liu[1] and Mark C. Hersam[1,2,3,4]*

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.



Key steps:

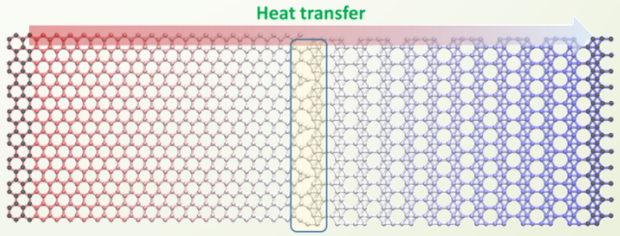
1. Ab-initio molecular dynamics simulations



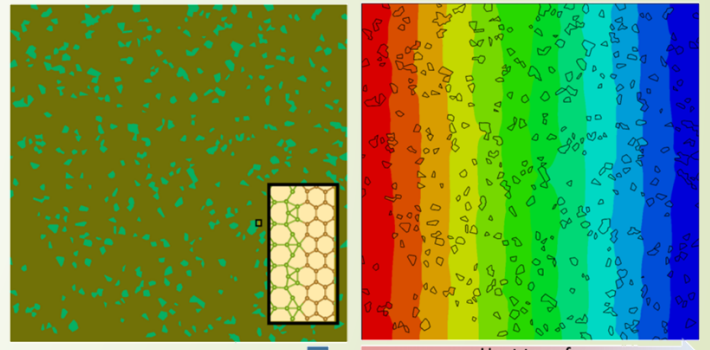
2. Machine-learning interatomic potentials

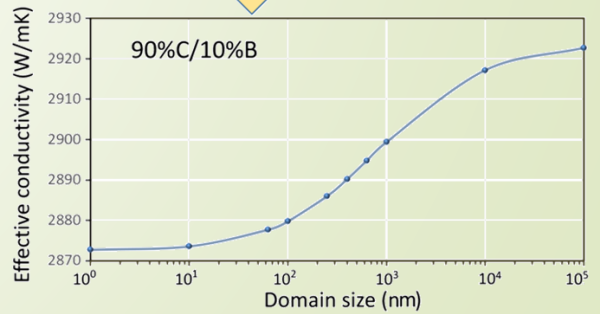
Moment tensor potentials (MTPs): $V(\boldsymbol{r}_i) = \sum_{j=1}^{m} \theta_j B_j(\boldsymbol{r}_i)$,

3. Classical molecular dynamics simulations



4. Finite element modeling of graphene/borophene heterostructures





B Mortazavi, et al. Materials Horizons 7 (2020), 2359-2367

First-principles multiscale modeling

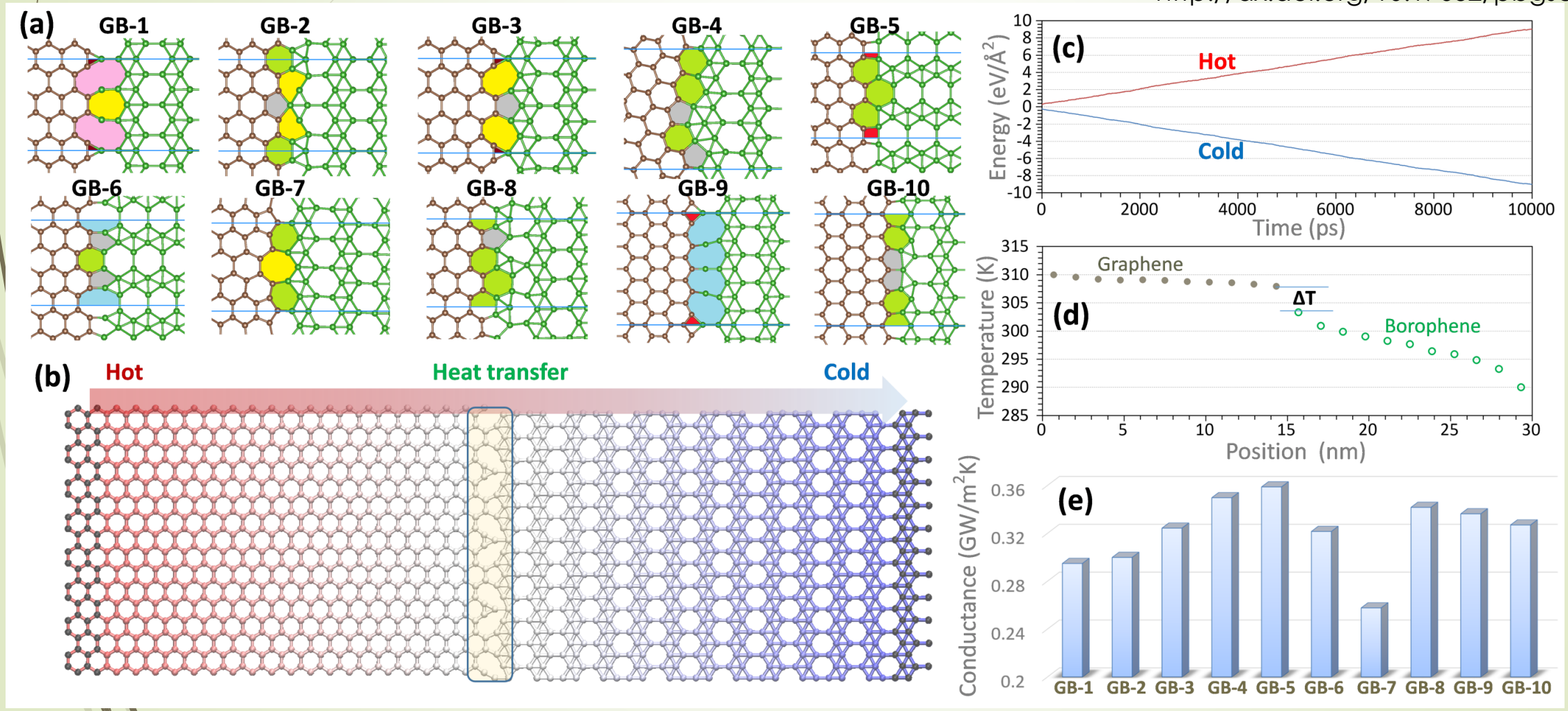
Thermal transport

Mendeley Data

This is your published dataset

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

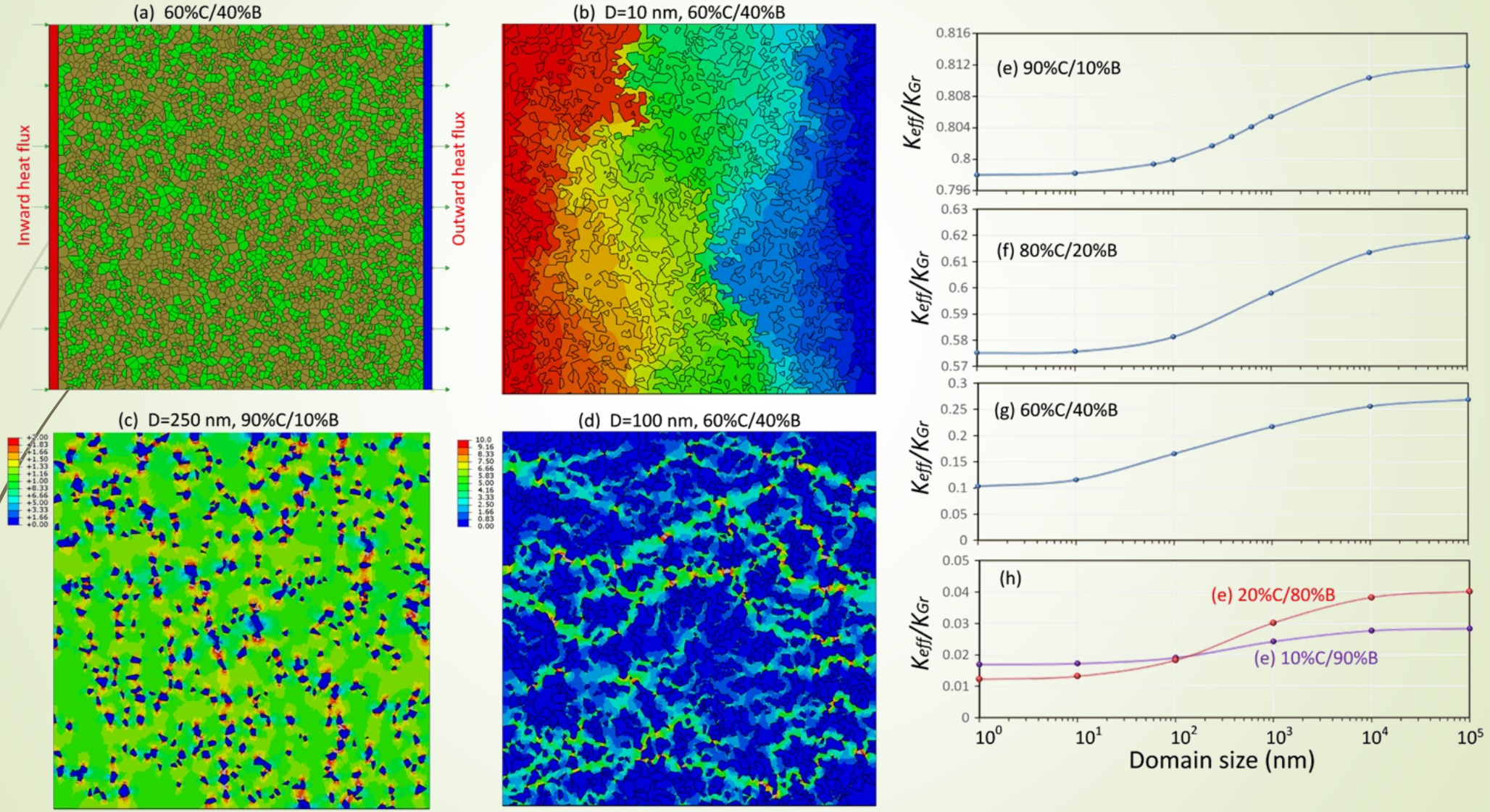
http://dx.doi.org/10.17632/pbgscy3ptg.1



B Mortazavi, et al. Materials Horizons 7 (2020), 2359-2367

First-principles multiscale modeling

Thermal transport

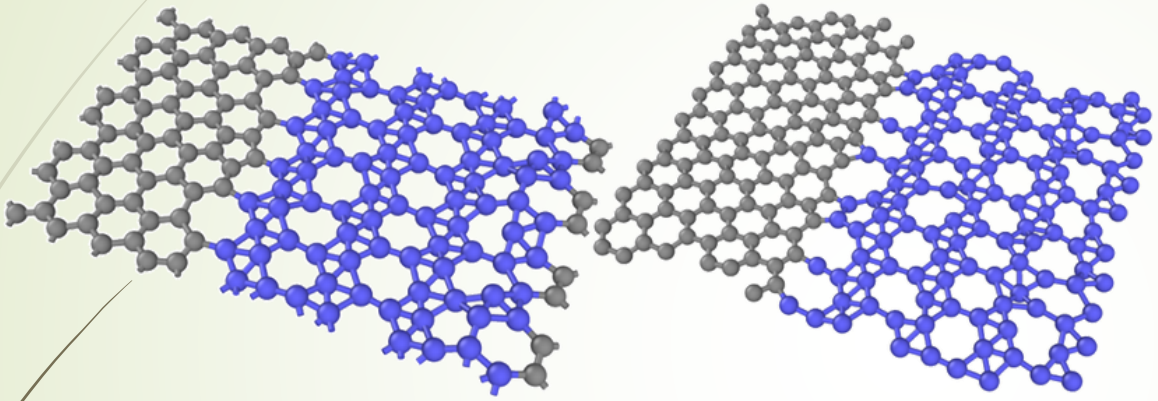


B Mortazavi, et al. Materials Horizons 7 (2020), 2359-2367

First-principles multiscale modeling

Mechanical properties

Step 1: Ab-initio calculations and dataset creation



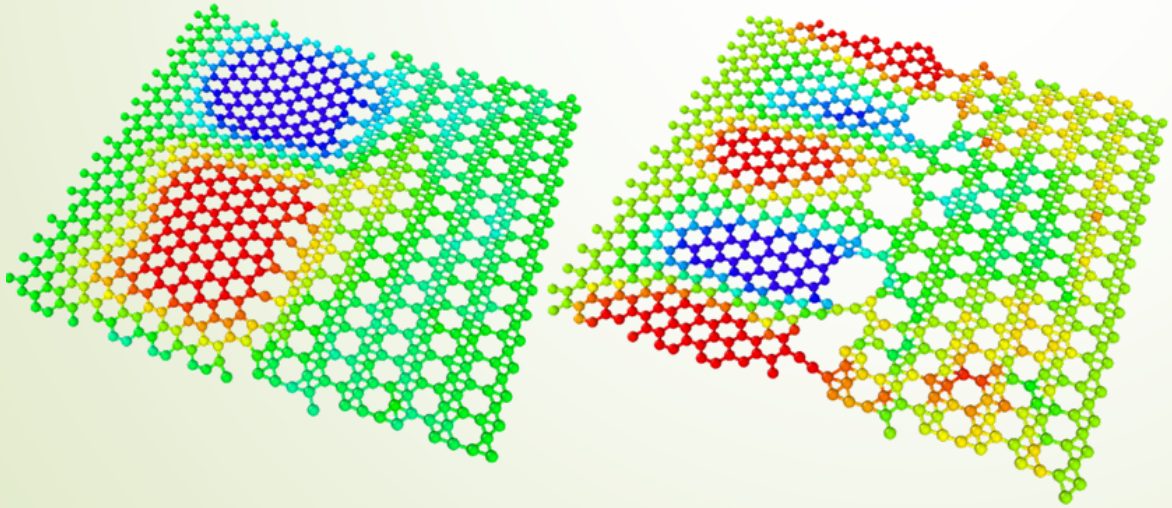
Step 2: Machine-learning interatomic potentials

Moment tensor potentials (MTPs):

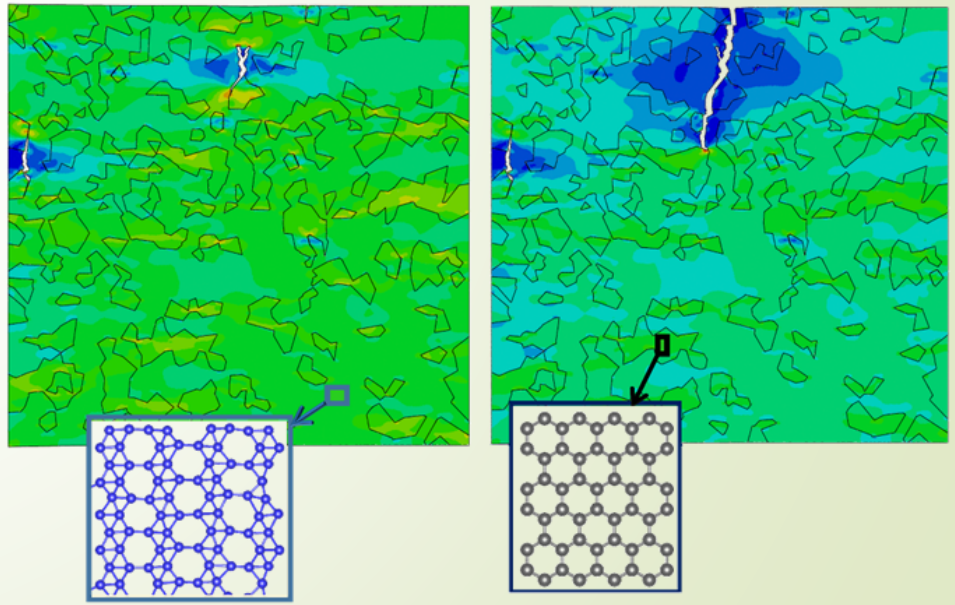
$$V(\mathfrak{n}_i) = \sum_{\alpha} \xi_{\alpha} B_{\alpha}(\mathfrak{n}_i),$$

$$M_{\mu,\nu}(\mathfrak{n}_i) = \sum_{j} f_{\mu}(|r_{ij}|, z_i, z_j)\, r_{ij} \otimes \ldots \otimes r_{ij},$$

Step 3: Classical molecular dynamics simulations



Step 4: Continuum finite element modeling



B Mortazavi, et al. Advanced Materials 33(2021), 2102807

First-principles multiscale modeling

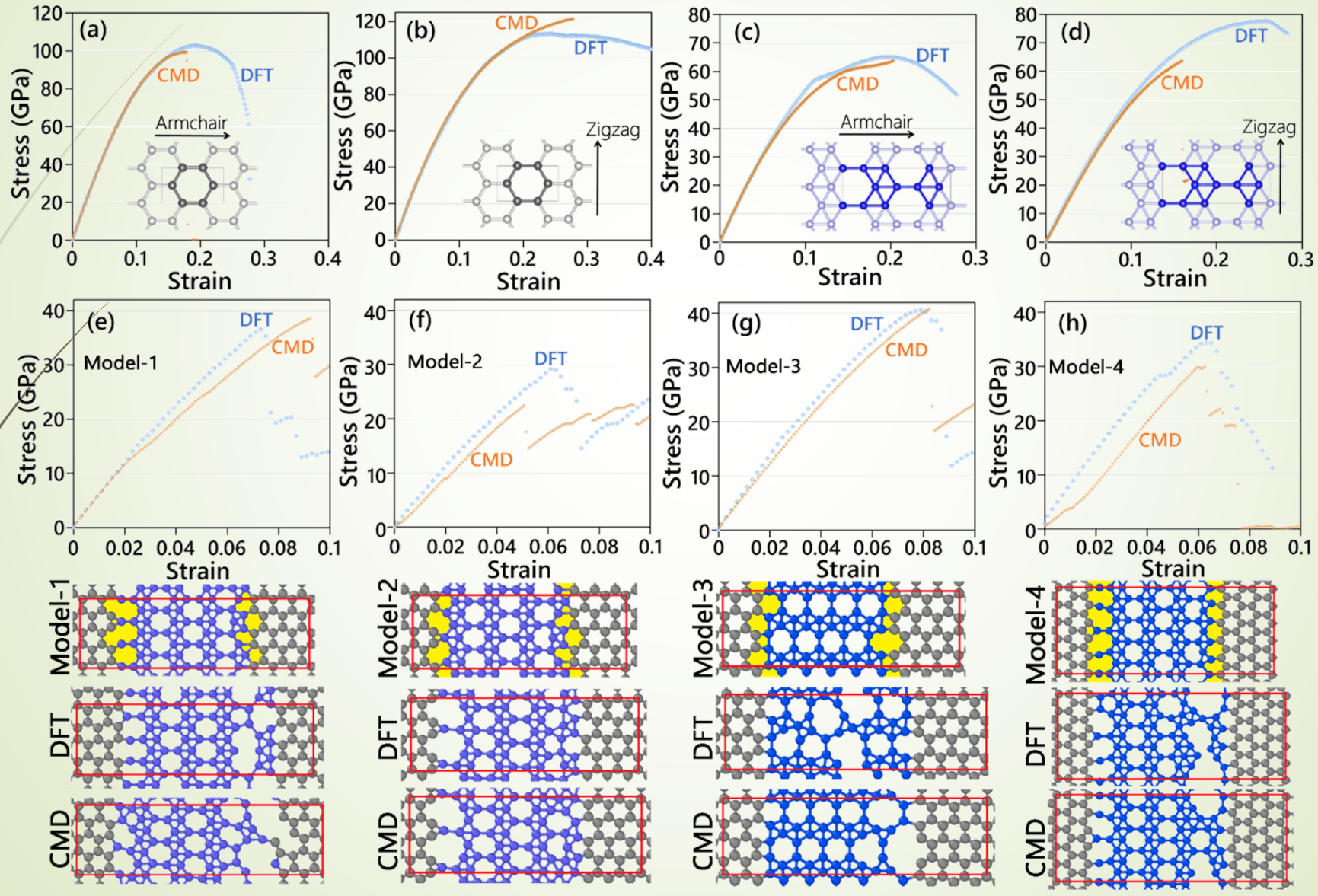
Mechanical properties

Mendeley Data

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

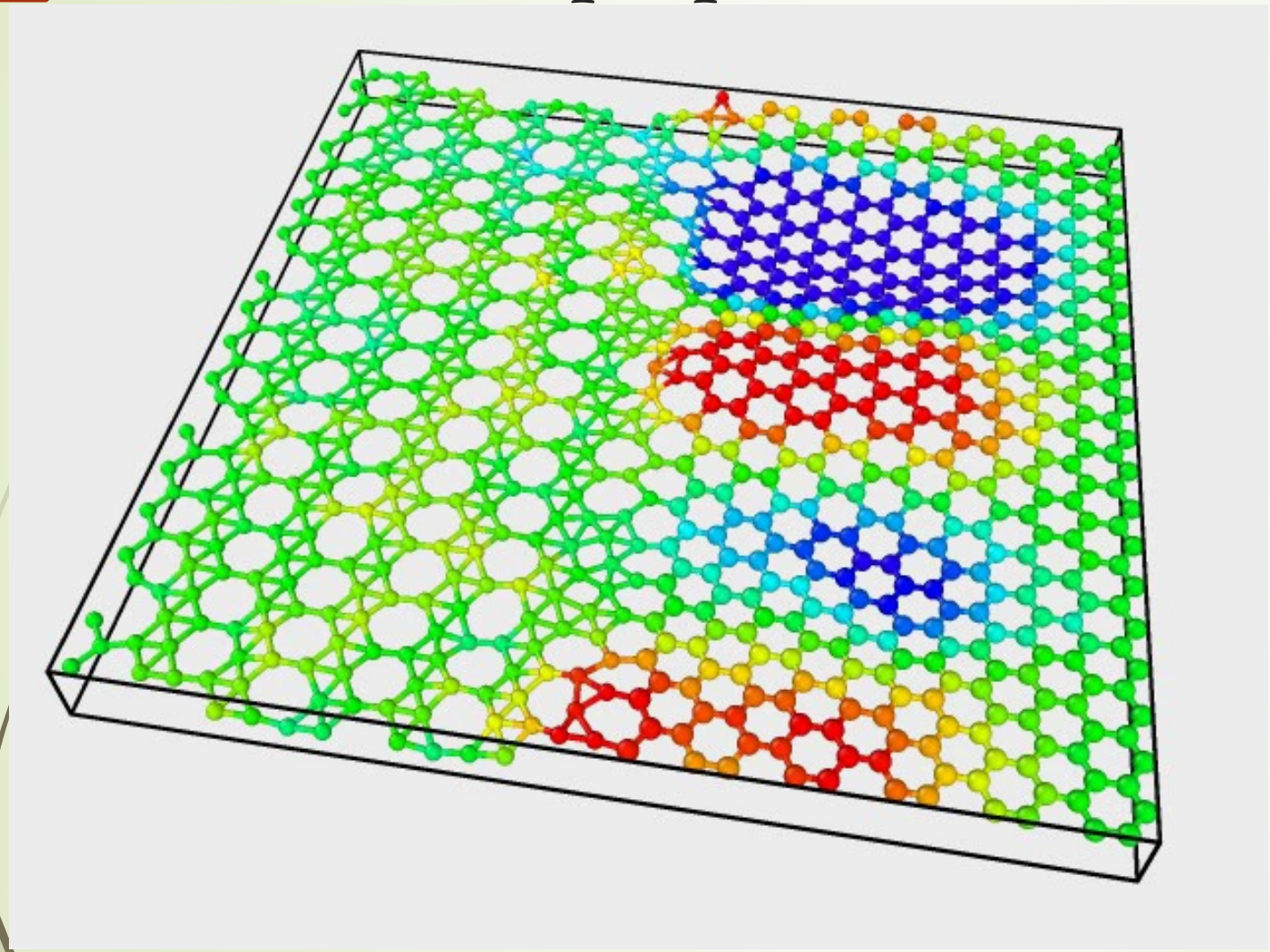
Published: 11 May 2021 | Version 1 | DOI: 10.17632/yrn7p7w37f.1
Contributor: Bohayra Mortazavi

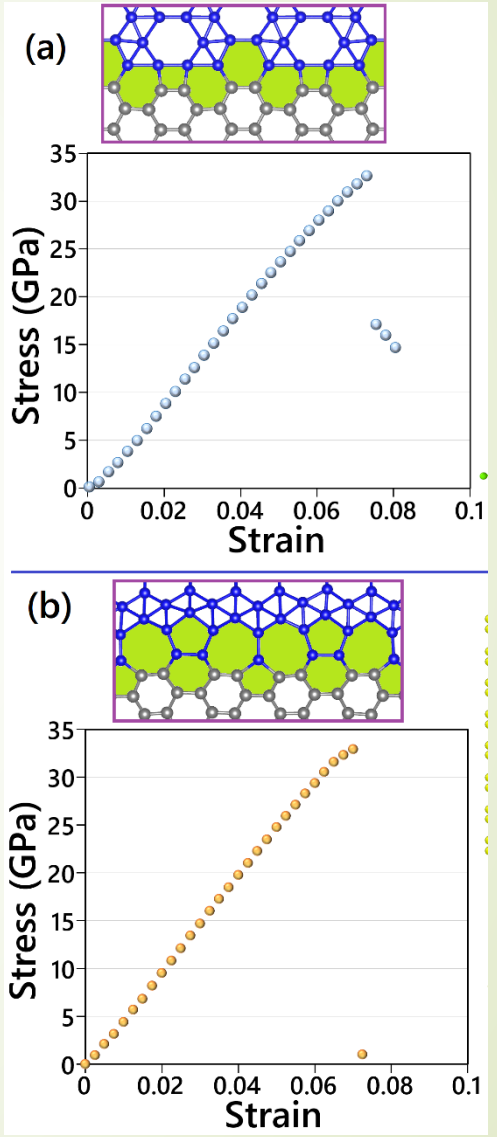
https://doi.org/10.17632/yrn7p7w37f.1



First-principles multiscale modeling

Mechanical properties





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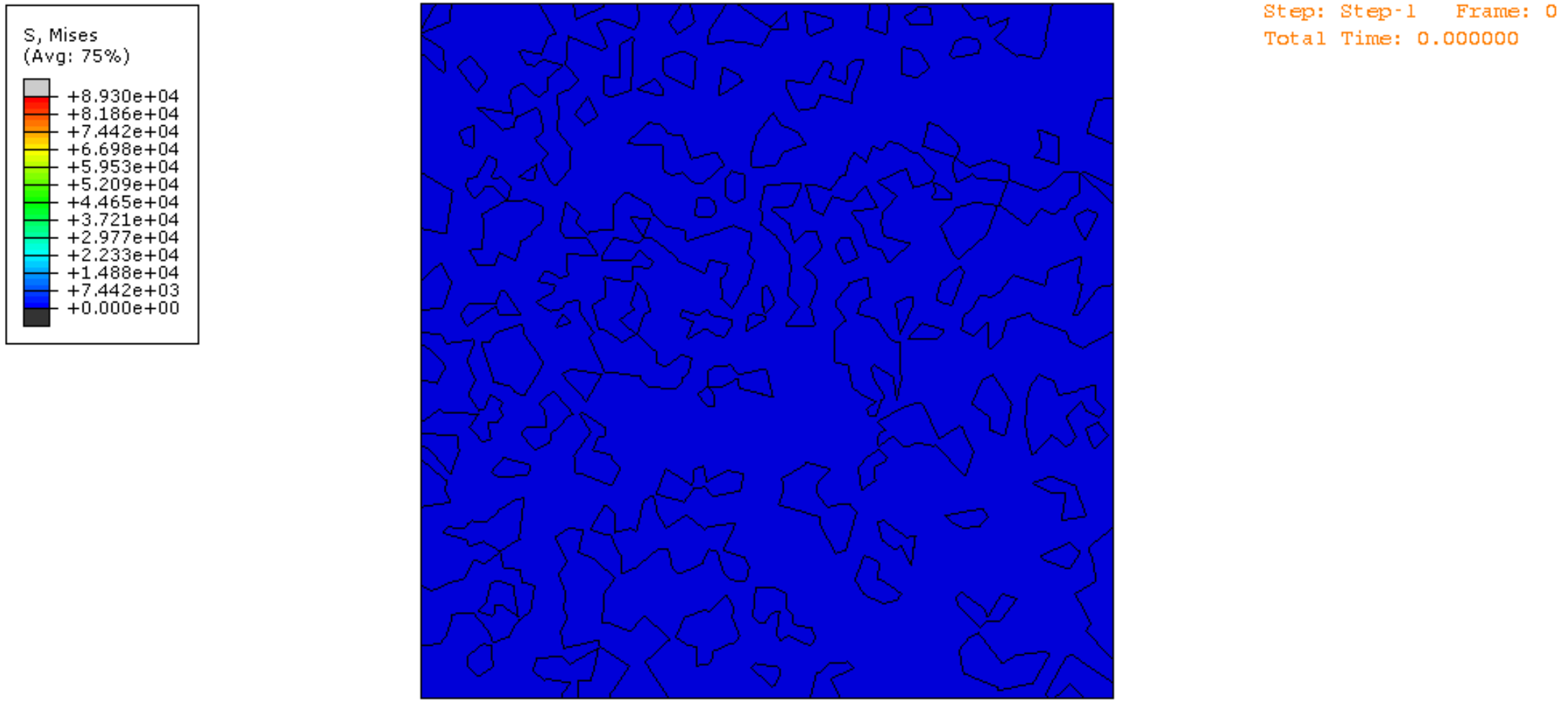
First-principles multiscale modeling

Mechanical properties



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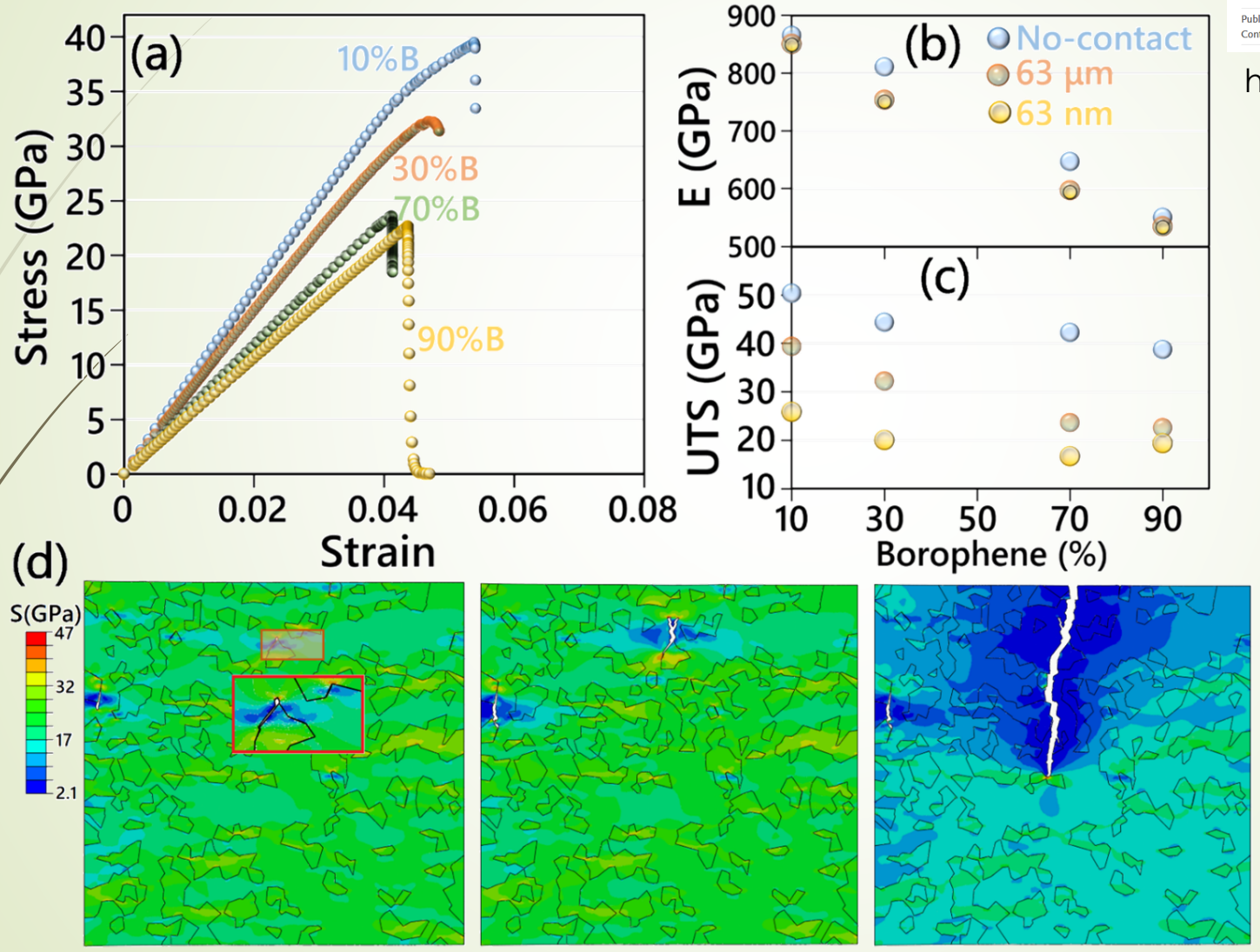
First-principles multiscale modeling

Mechanical properties



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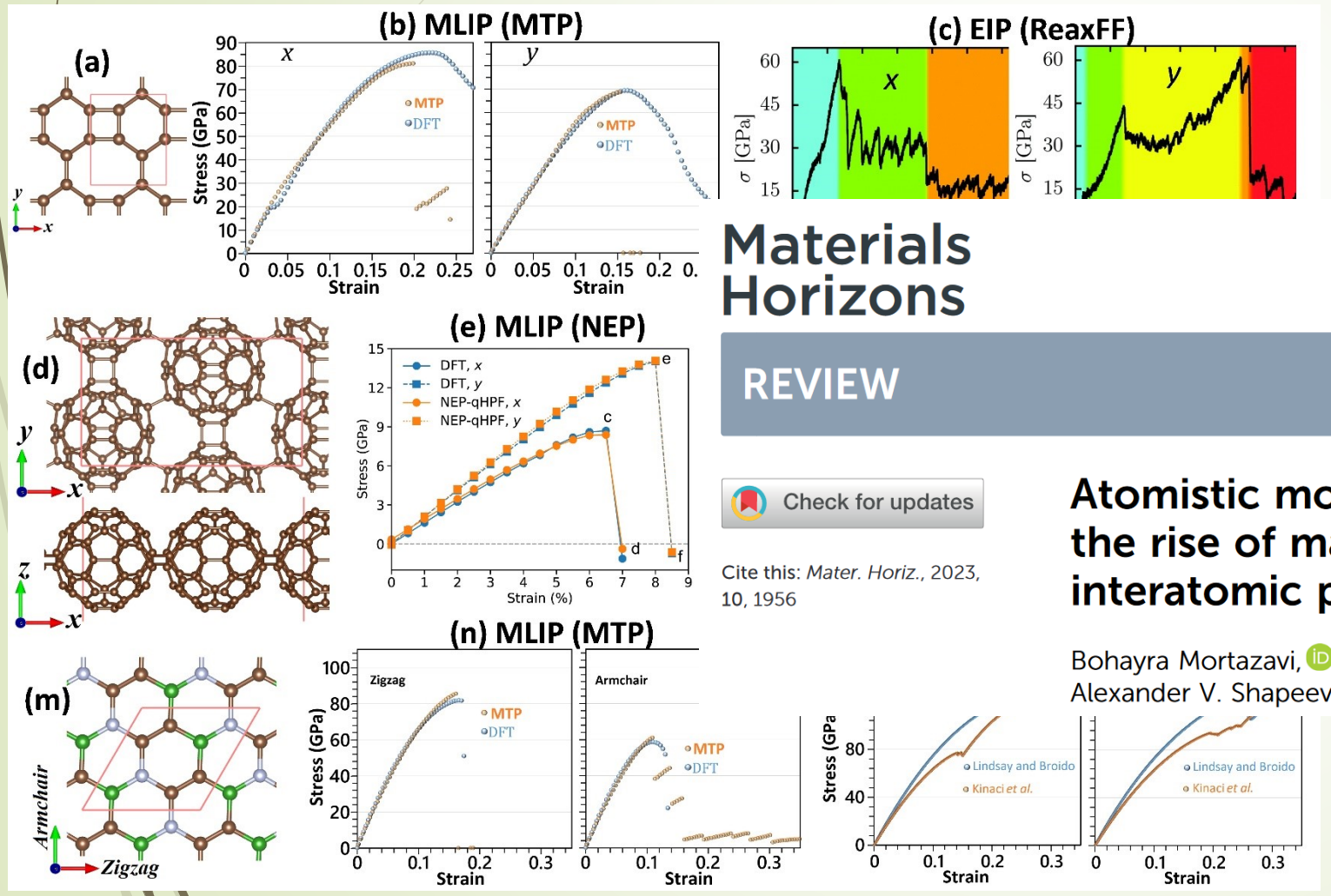
http://dx.doi.org/10.17632/pbgscy3ptg.1

First-principles multiscale modeling

Misguiding of empirical interatomic potentials

Considering novel 2D systems



Materials Horizons

REVIEW

Check for updates

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

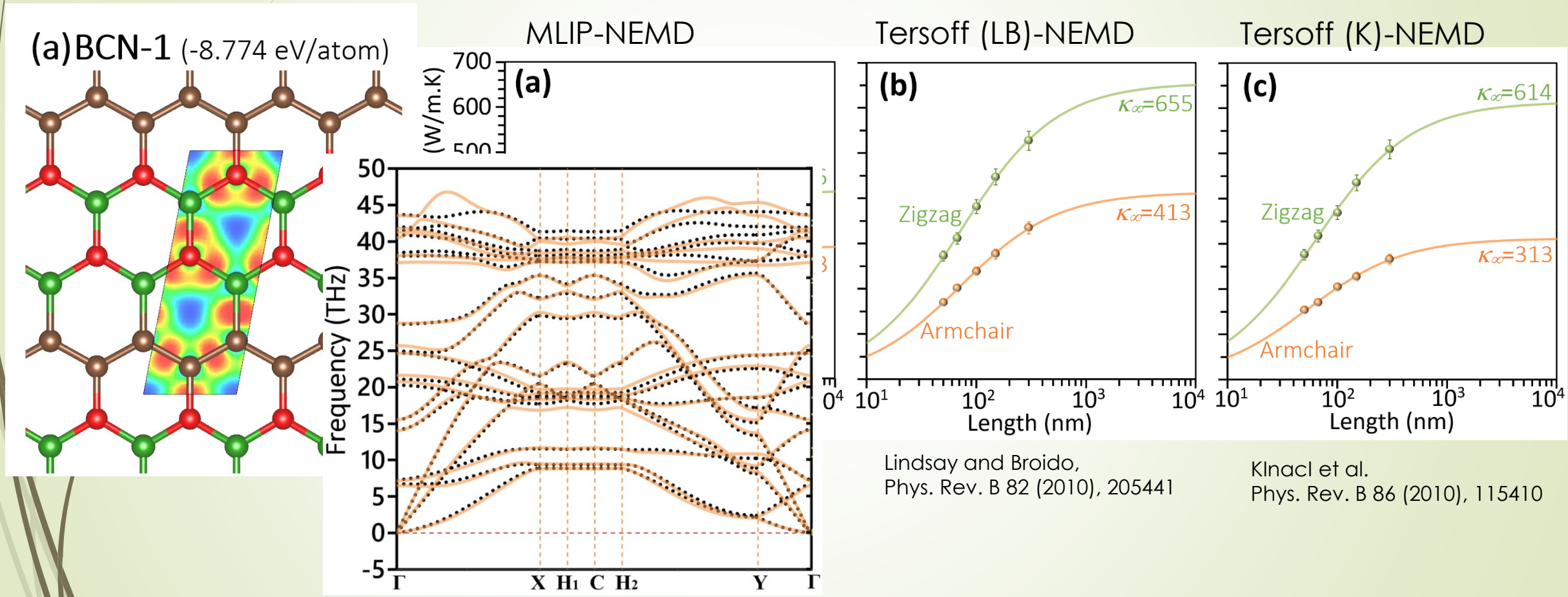
Atomistic modeling of the mechanical properties: the rise of machine learning interatomic potentials

Bohayra Mortazavi, *[ab] Xiaoying Zhuang,*[ac] Timon Rabczuk[d] and Alexander V. Shapeev*[e]

First-principles multiscale modeling

Misguiding of empirical interatomic potentials

Comparison with empirical interatomic potentials



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

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

B Mortazavi, et al. Carbon 200 (2022), 500-509

Thanks a lot for your attentions

Questions?