



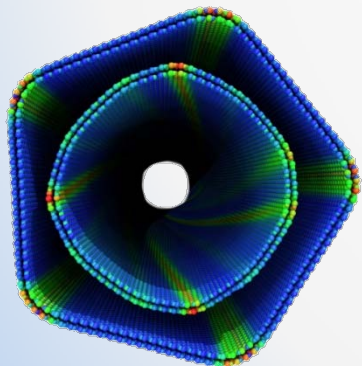
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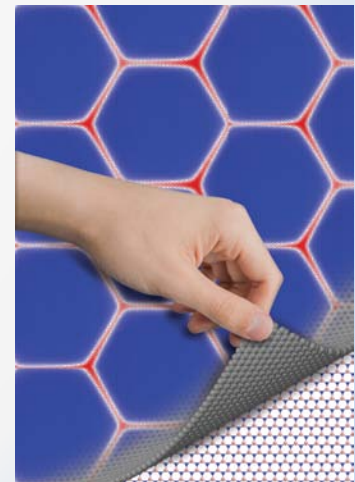


TEL AVIV אוניברסיטת  
UNIVERSITY תל אביב

# Modeling Inter-layer Interactions in Layered Materials



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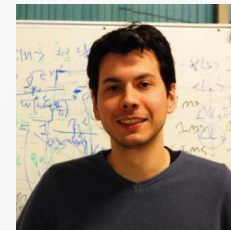
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Yaron Itkin  
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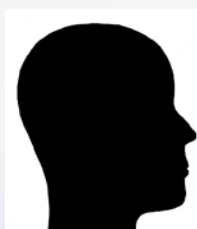
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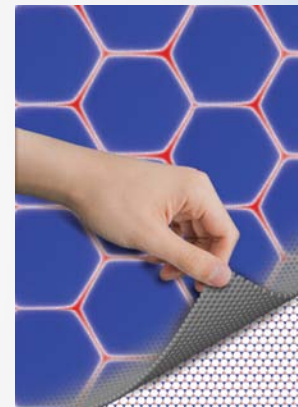
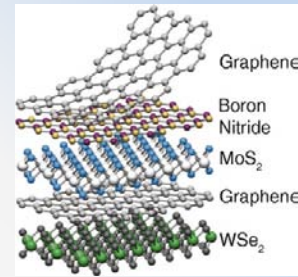


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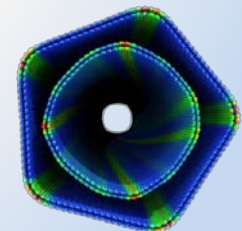
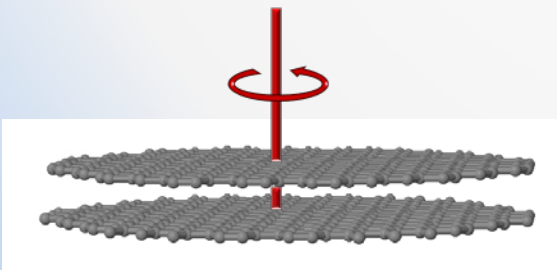


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Adi Blumberg,  
Uri Keshet,  
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Katherine Akulov .

# Outline

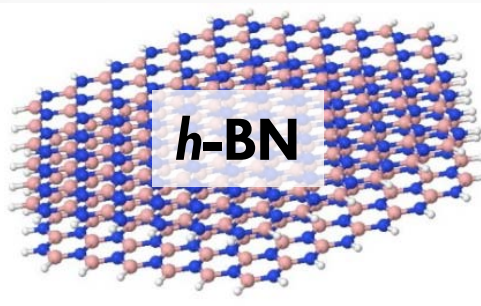
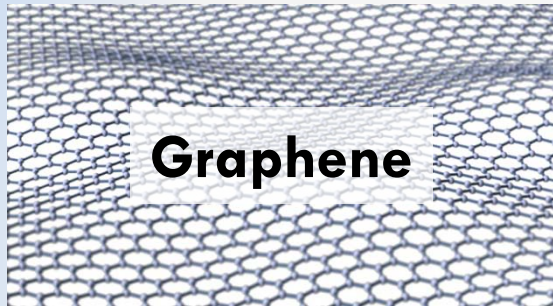


- Why layered materials?
- Levels of modeling.
- Classical intra- and inter-layer force fields.
- Applications of classical force-fields:
  - ✓ Structure of Graphene/*h*-BN hetero-structures.
  - ✓ ~~Robust superlubricity in layered hetero-junctions.~~
  - ✓ Faceting in multi-walled nanotubes.
  - ✓ Inter-wall friction in CNTs and BNNTs.
- ~~Electron transport across twisted graphene interfaces.~~
- Summary and outlook.

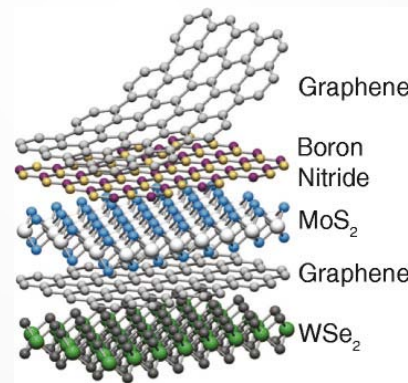


# Layered Materials at the Nanoscale

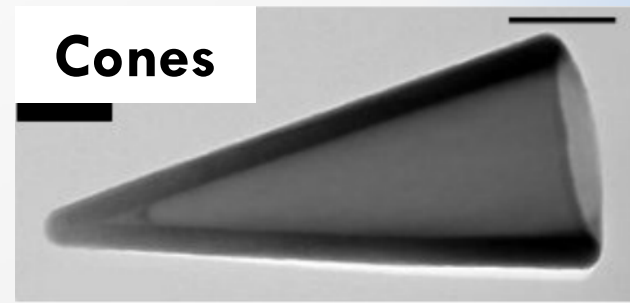
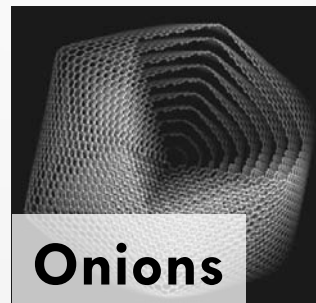
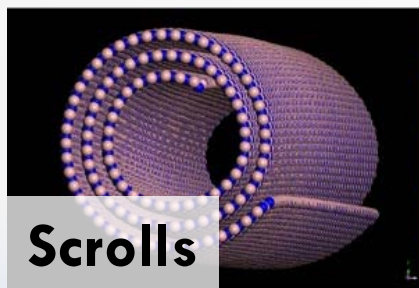
- A large family of materials



- Diverse structures



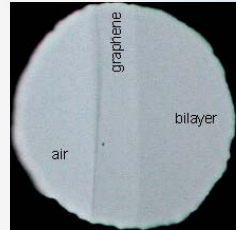
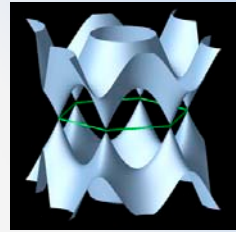
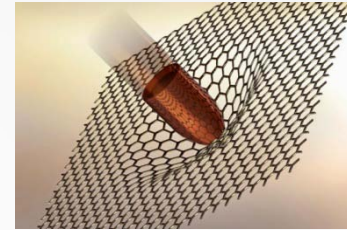
**Sheets**



# Layered Materials at the Nanoscale

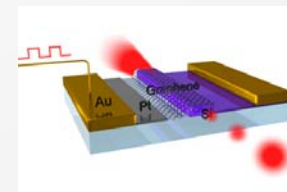
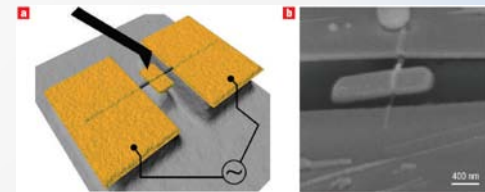
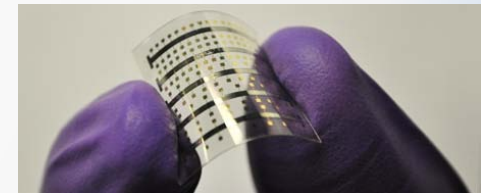
## Unique properties

- Controllable electronic properties.
- Enhanced mechanical rigidity.
- Structural anisotropy.
- Optical activity.
- Efficient heat transport.
- ...



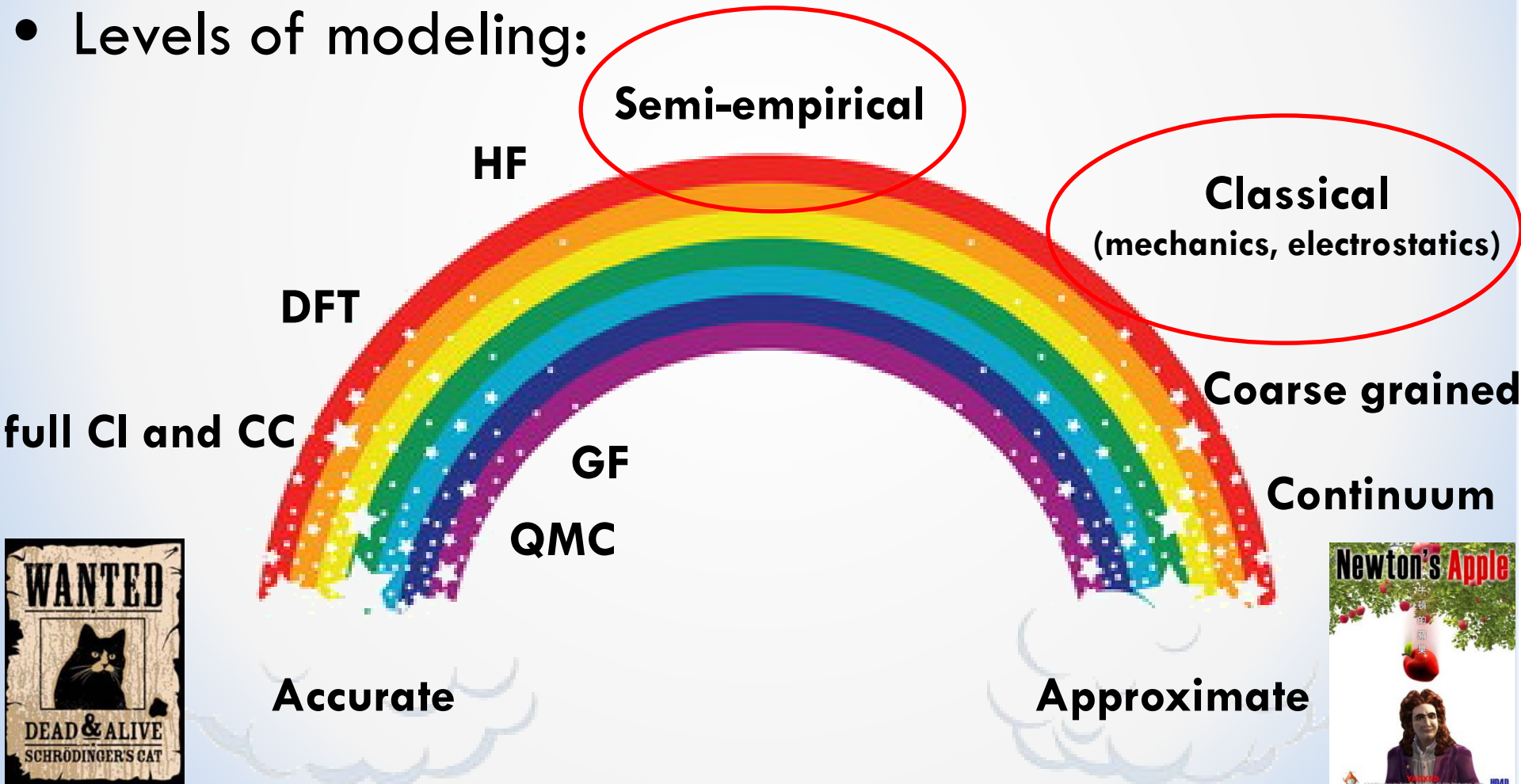
## Possible applications

- Electronics and spintronics devices.
- Nano-electromechanical systems.
- Optics and communication.
- Tribology and solid lubrication.
- ...

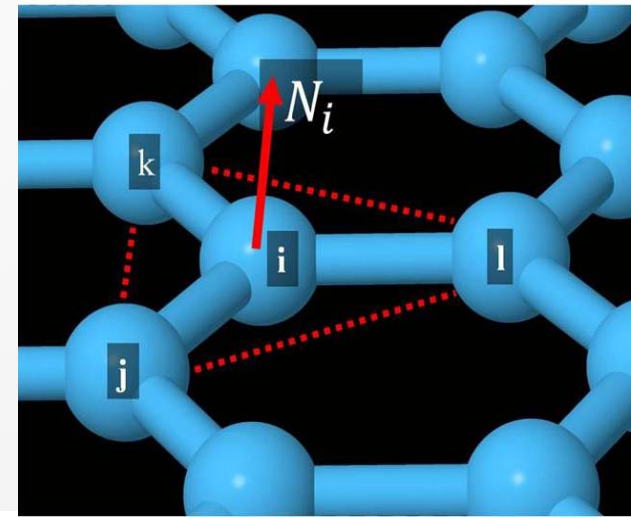


# Modeling Nanoscale Layered Materials

- At the nanoscale modeling and simulations are accurate and efficient.
- Levels of modeling:



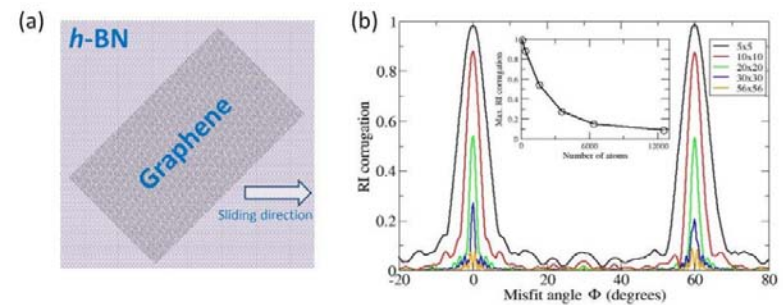
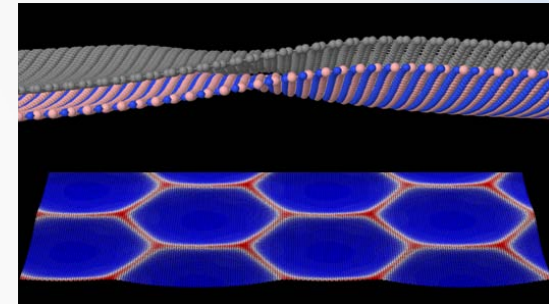
# Classical Force-Fields Construction



# Classical Force-Fields

- Classical force-fields can be used to model many properties of layered materials:

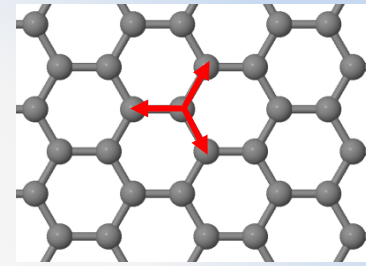
- ✓ Structural
- ✓ Mechanical
- ✓ Tribological
- ✓ Heat transport
- ✓ Chemical



- Layered materials are anisotropic by nature.
- Calls for a separate treatment of intra- and inter-layer interactions.



# Intra-Layer Potentials



- Intra-layer interactions are often modeled via:

✓ Bonded two-body interactions (distances).  $V_{ij} = k_{ij} (r_{ij} - r_0)^2$

✓ Bonded three-body interactions (angles).  $V_{ijk} = k_{ijk} [\cos(\theta_{ijk}) - \cos(\theta_0)]^2$

✓ Bonded four-body interactions (dihedrals and Improper).

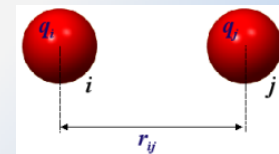
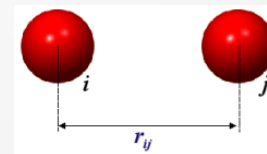
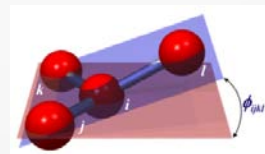
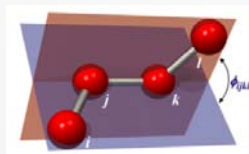
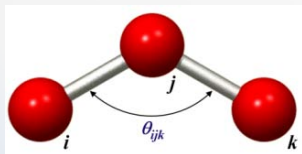
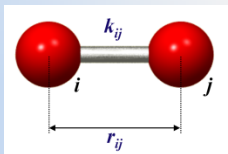
✓ Van der Waals.  $V_{vdw} = 4\epsilon \left[ \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left( \frac{\sigma_{ij}}{r_{ij}} \right)^6 \right]$   $V_{ijkl} = k_{ijkl} [1 + \cos(n_{ijkl}\phi_{ijkl} - \phi_0)]^2$

✓ Electrostatics.

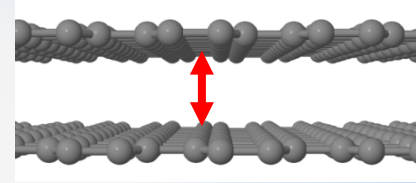
$$V_{Coul} = \frac{kq_i q_j}{r_{ij}} \quad V_{ijkl} = k_{ijkl} (\phi_{ijkl} - \phi_0)^2$$

- Examples:

Tersoff, Brenner, AIREBO, REAXFF, AMBER, CHARMM, MM4, ...



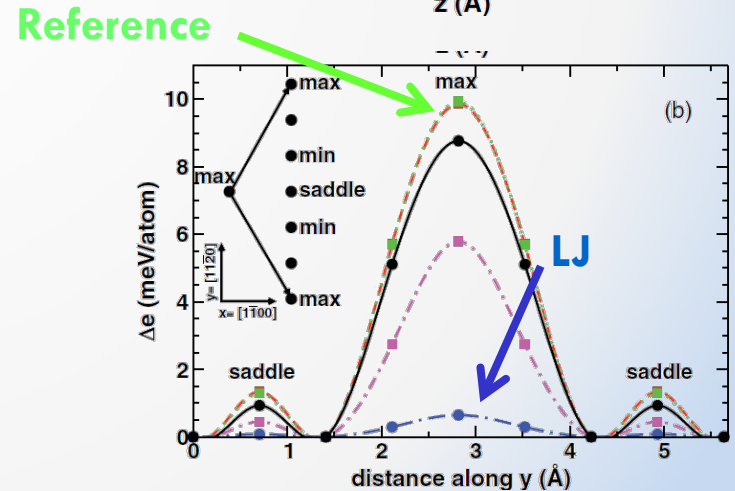
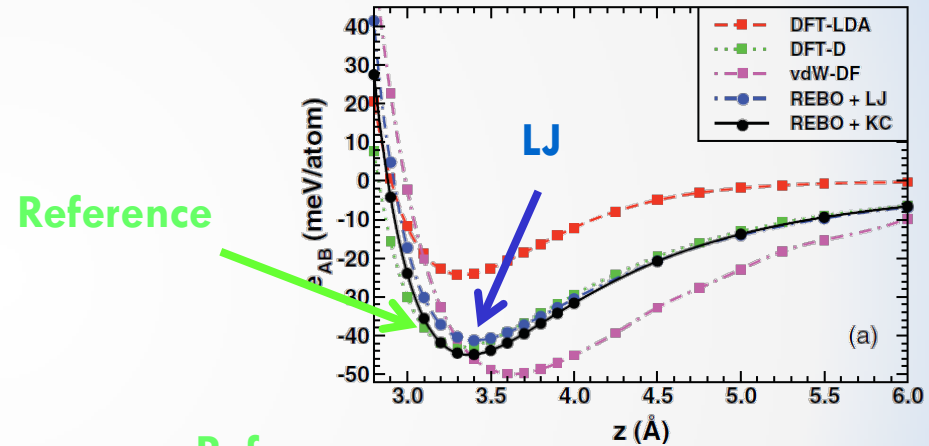
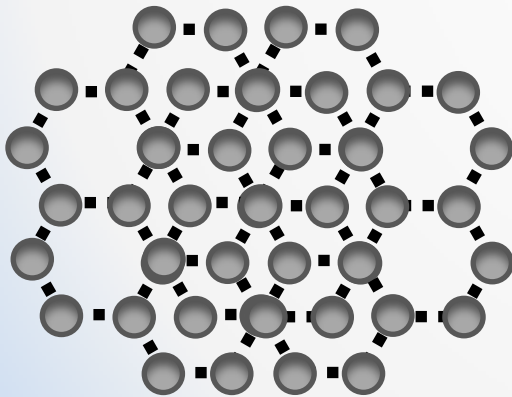
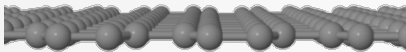
# Inter-Layer Potentials



- Inter-layer interactions often include:
  - ✓ Isotropic long-range dispersive attractions.
  - ✓ (An)isotropic short-range Pauli repulsions.
  - ✓ Electrostatics.
- Examples:  
Lennard-Jones/Morse, Kolmogorov-Crespi, *h*-BN ILP, *h*-BN/graphene ILP
- A **range-separation cutoff** or a **clear layer separation** is required to apply the two terms simultaneously.

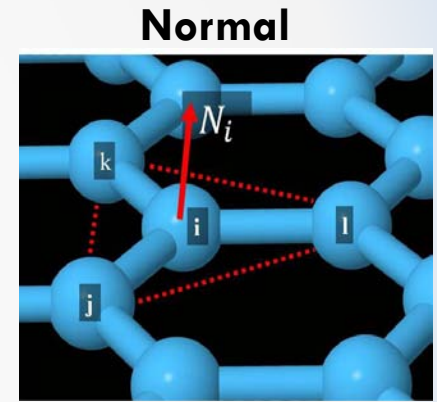
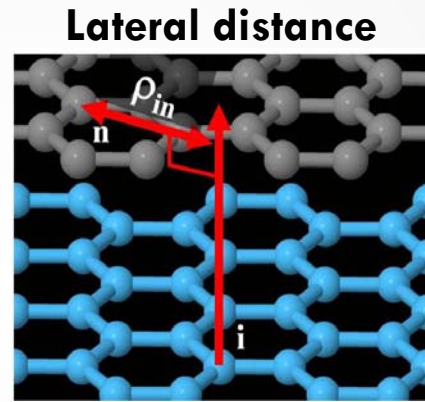
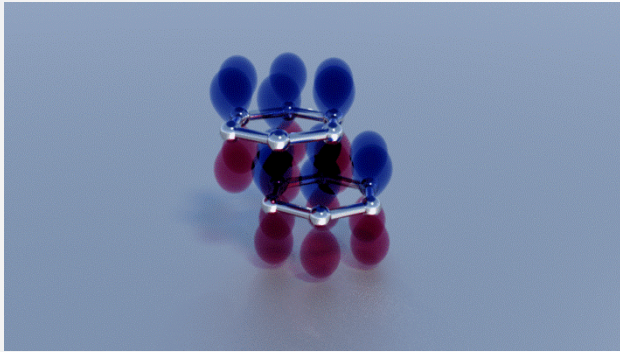
# Isotropic Interlayer Potential for Graphene

- Isotropic potentials often provide a good description of the interlayer binding energy curve.
- However it predicts too shallow sliding energy curves.



# Anisotropic Interlayer Potential for Graphene Kolmogorov & Crespi (KC)

- **Pauli repulsions** depend on the **lateral distance** between two atoms on adjacent layers as they cross each-other during the sliding process.



$$V(\mathbf{r}_{ij}, \mathbf{n}_i, \mathbf{n}_j) = e^{-\lambda(r_{ij}-z_0)} [C + f(\rho_{ij}) + f(\rho_{ji})] - A \left( \frac{r_{ij}}{z_0} \right)^{-6}$$

Repulsive Morse-like term

Anisotropic Gaussian term

Attractive LJ-like term.

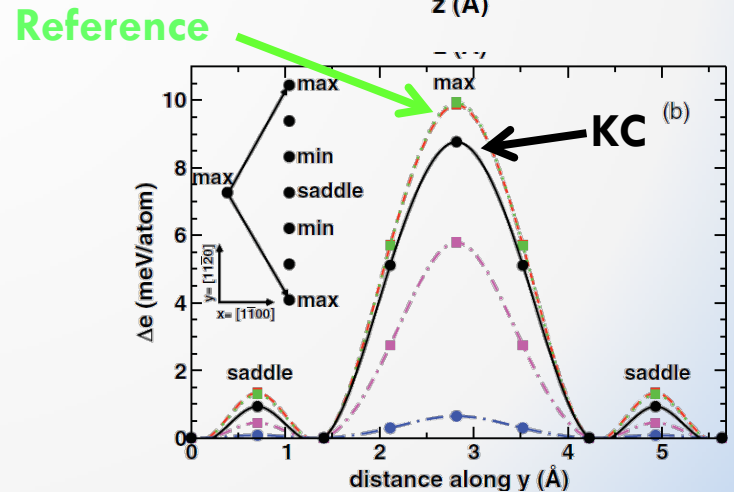
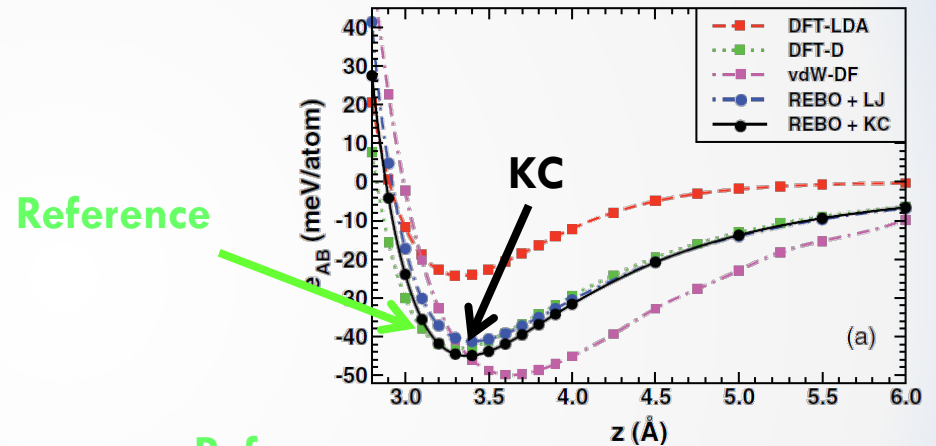
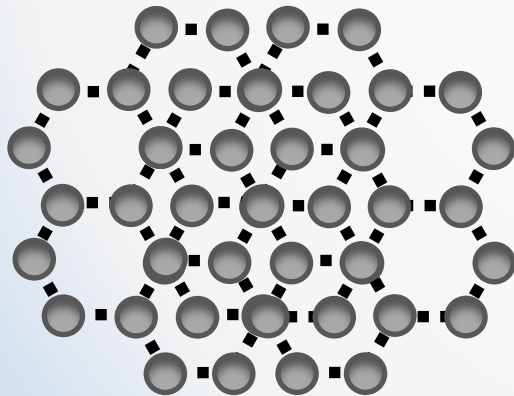
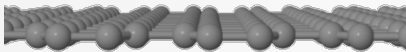
$$\rho_{ij}^2 = r_{ij}^2 - (\mathbf{n}_i \mathbf{r}_{ij})^2,$$

$$\rho_{ji}^2 = r_{ij}^2 - (\mathbf{n}_j \mathbf{r}_{ij})^2,$$

$$f(\rho) = e^{-(\rho/\delta)^2} \sum C_{2n} (\rho/\delta)^{2n}.$$

# Anisotropic Interlayer Potential for Graphene Kolmogorov & Crespi (KC)

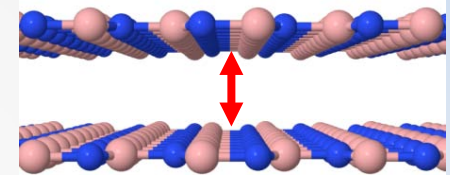
- KC can describe both motions simultaneously for **graphene**.



# Anisotropic Interlayer Potential for *h*-BN

## *h*-BN ILP

- *h*-BN ILP follows the spirit of the KC potential.
- vdW + repulsion:



$$E_{vdW} = e \left( \alpha_{ij} \left( 1 - \frac{r_{ij}}{R_{ij}} \right) \right) \left[ \varepsilon_{ij} + C \left( e^{-\left( \frac{\rho_{ij}}{\gamma_{ij}} \right)^2} + e^{-\left( \frac{\rho_{ji}}{\gamma_{ij}} \right)^2} \right) \right] - \frac{1}{1 + e^{-d \left( \frac{r_{ij}}{S_r r_{eff}} - 1 \right)}} \left( \frac{c_6}{r_{ij}^6} \right)$$

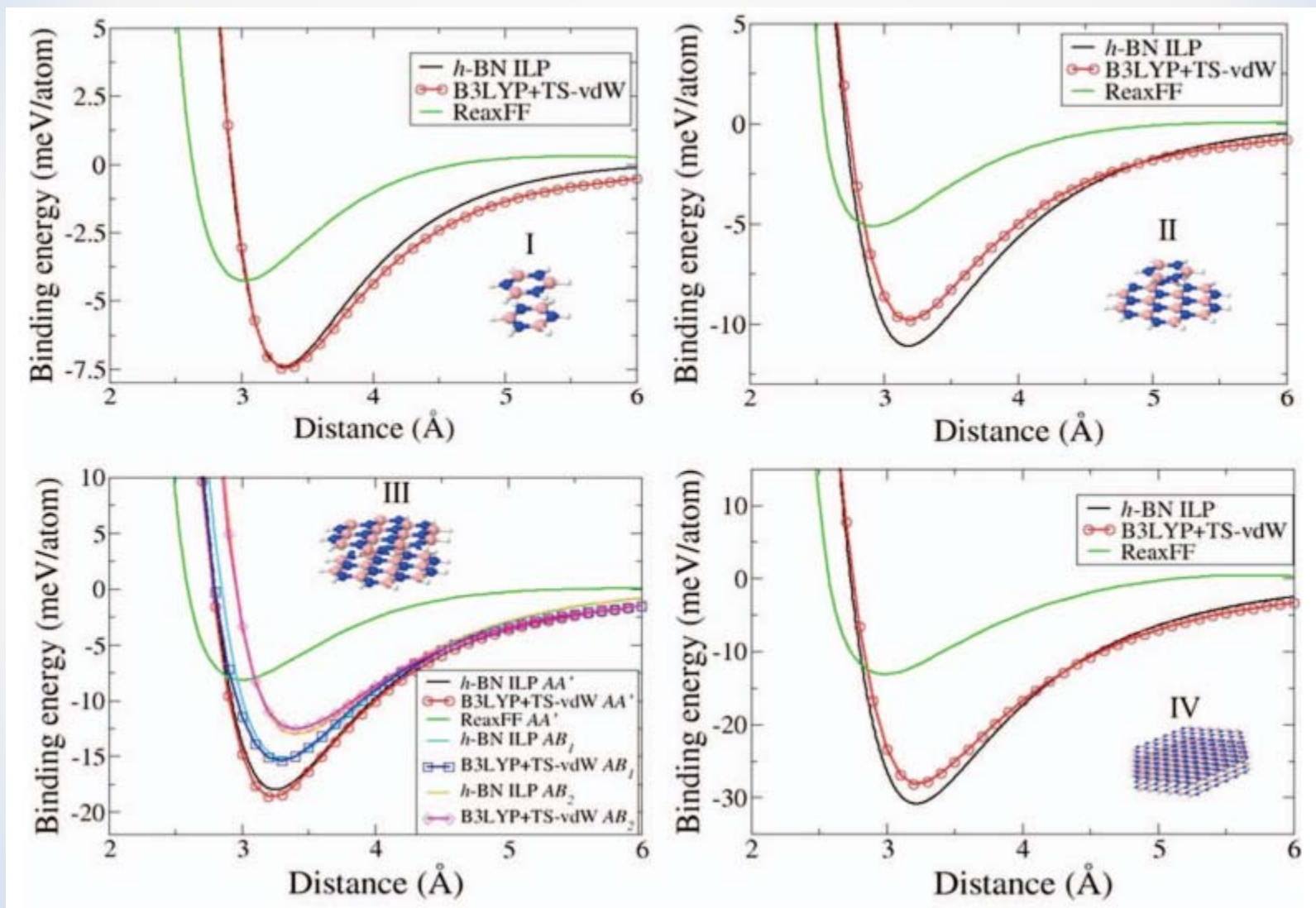
Repulsive Morse-like term    Anisotropic Gaussian term    Short-range Fermi-Dirac damping term    Attractive LJ-like term.

- Coulomb interactions between partially charged atomic centers:

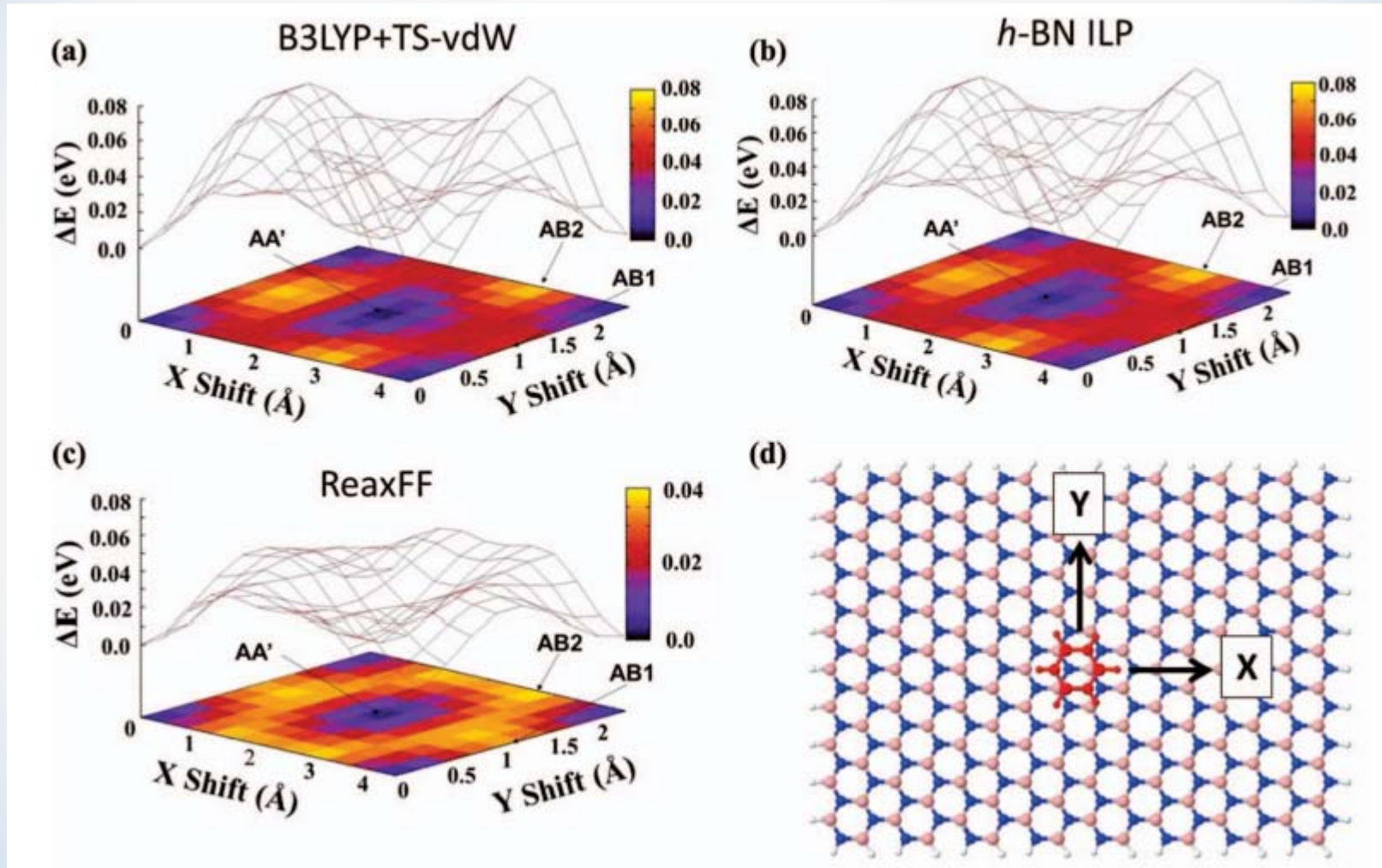
$$E_{Coul} = k \frac{q_i q_j}{\sqrt[3]{r_{ij}^3 + \left( \frac{1}{\lambda_{ij}} \right)^3}}$$

- vdW parameters taken from TS-vdW calculations.
- All parameters fine tuned against TS-vdW DFT.

# *h*-BN ILP performance - Binding

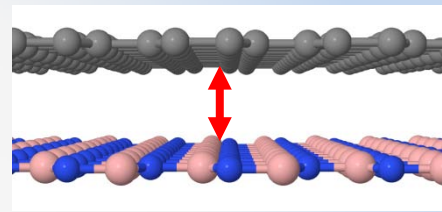


# *h*-BN ILP performance - Sliding

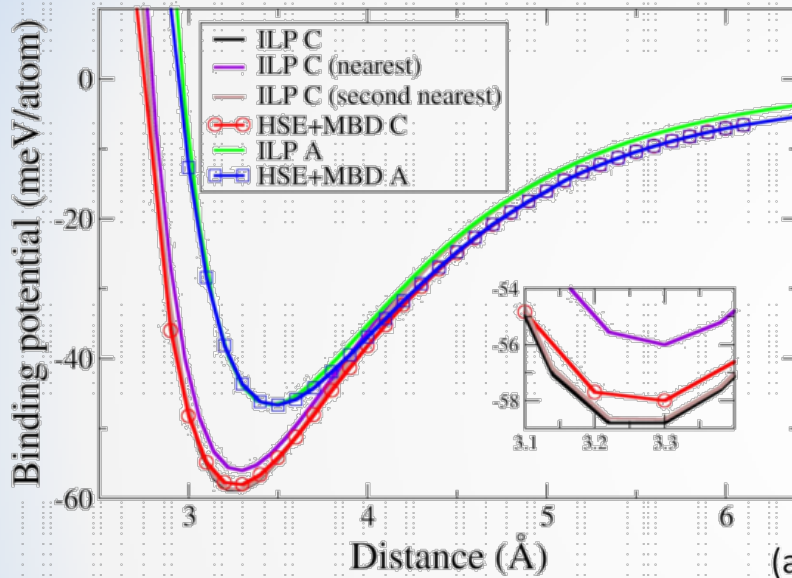




# Graphene/*h*-BN ILP

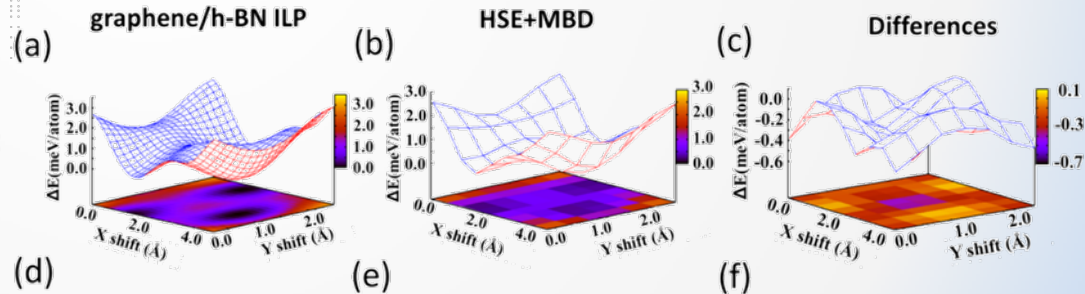


- Same functional form as the *h*-BN ILP without Coulomb interactions.

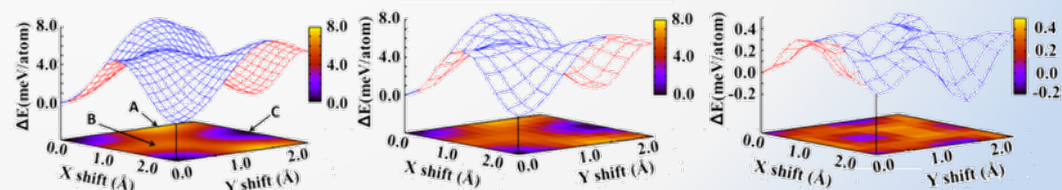


**Binding energy of bulk graphene/*h*-BN alternating stacks.**

Benzene/*h*BN



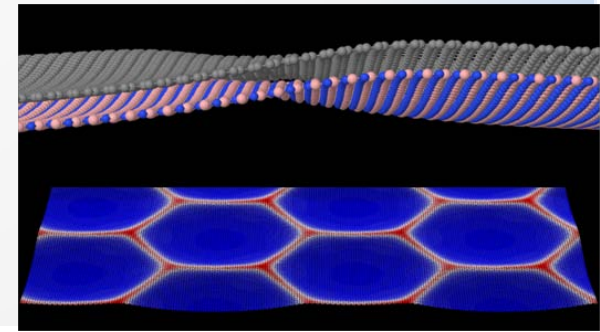
Periodic  
graphene/*h*-BN



**Sliding energy landscapes**

# Classical Force-Fields Applications

## Graphene/*h*-BN Heterojunctions



# Graphene/*h*-BN Hetero-Structures

LETTERS

PUBLISHED ONLINE: 14 JULY 2013 | DOI: 10.1038/NMAT2695

nature  
materials

## Epitaxial growth of single-domain graphene on hexagonal boron nitride

Wei Yang<sup>1</sup>, Guorui Chen<sup>2</sup>, Zhiwen Shi<sup>1</sup>, Cheng-Cheng Liu<sup>1,3</sup>, Lianchang Zhang<sup>1,4</sup>, Guibai Xie<sup>1</sup>, Meng Cheng<sup>1</sup>, Duoming Wang<sup>1</sup>, Rong Yang<sup>1</sup>, Dongxia Shi<sup>1</sup>, Kenji Watanabe<sup>5</sup>, Takashi Taniguchi<sup>5</sup>, Yugui Yao<sup>3</sup>, Yuanbo Zhang<sup>2</sup> and Guangyu Zhang<sup>1\*</sup>

## Field-Effect Tunneling Transistor Based on Vertical Graphene Heterostructures

L. Britnell<sup>1</sup>, R. V. Gorbachev<sup>2</sup>, R. Jalil<sup>2</sup>, B. D. Belle<sup>2</sup>, F. Schedin<sup>2</sup>, A. Mishchenko<sup>1</sup>, T. Georgiou<sup>1</sup>, M. I. Katsnelson<sup>3</sup>, L. Eaves<sup>4</sup>, S. V. Morozov<sup>5</sup>, N. M. R. Peres<sup>6,7</sup>, J. Leist<sup>8</sup>, A. K. Geim<sup>1,2\*</sup>, K. S. Novoselov<sup>1\*</sup>, L. A. Ponomarenko<sup>1\*</sup>

LETTERS

PUBLISHED ONLINE: 22 AUGUST 2010 | DOI: 10.1038/NANO.2010.172

nature  
nanotechnology

## Boron nitride substrates for high-quality graphene electronics

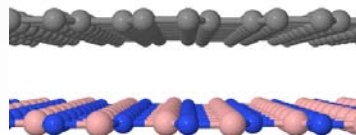
C. R. Dean<sup>1,2\*</sup>, A. F. Young<sup>1</sup>, I. Meric<sup>1</sup>, C. Lee<sup>4,5</sup>, L. Wang<sup>2</sup>, S. Sorgenfrei<sup>1</sup>, K. Watanabe<sup>6</sup>, T. Taniguchi<sup>6</sup>, P. Kim<sup>3</sup>, K. L. Shepard<sup>1</sup> and J. Hone<sup>2\*</sup>

LETTER

doi:10.1038/nature11408

## Graphene and boron nitride lateral heterostructures for atomically thin circuitry

Mark P. Levendorf<sup>1\*</sup>, Cheol-Joo Kim<sup>1\*</sup>, Lola Brown<sup>1</sup>, Pinshane Y. Huang<sup>2</sup>, Robin W. Havener<sup>2</sup>, David A. Muller<sup>2,3</sup> & Jiwoong Park<sup>1,3</sup>



LETTERS

PUBLISHED ONLINE: 22 JUNE 2015 | DOI: 10.1038/NANO.2015.131

nature  
nanotechnology

## Graphene on hexagonal boron nitride as a tunable hyperbolic metamaterial

S. Dai<sup>1</sup>, Q. Ma<sup>2</sup>, M. K. Liu<sup>1,3</sup>, T. Andersen<sup>2</sup>, Z. Fei<sup>1</sup>, M. D. Goldflam<sup>1</sup>, M. Wagner<sup>1</sup>, K. Watanabe<sup>4</sup>, T. Taniguchi<sup>4</sup>, M. Thiemens<sup>5</sup>, F. Keilmann<sup>6</sup>, G. C. A. M. Janssen<sup>7</sup>, S-E. Zhu<sup>7</sup>, P. Jarillo-Herrero<sup>2</sup>, M. M. Fogler<sup>1</sup> and D. N. Basov<sup>1\*</sup>

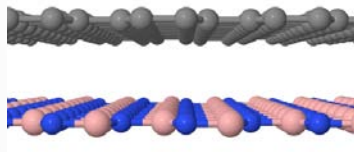
LETTERS

PUBLISHED ONLINE: 13 FEBRUARY 2011 | DOI: 10.1038/NMAT2968

nature  
materials

## Scanning tunnelling microscopy and spectroscopy of ultra-flat graphene on hexagonal boron nitride

Jiamin Xue<sup>1</sup>, Javier Sanchez-Yamagishi<sup>2</sup>, Danny Bulmash<sup>2</sup>, Philippe Jacquod<sup>1,3</sup>, Aparna Deshpande<sup>1,1</sup>, K. Watanabe<sup>4</sup>, T. Taniguchi<sup>4</sup>, Pablo Jarillo-Herrero<sup>2</sup> and Brian J. LeRoy<sup>1\*</sup>



LETTER

doi:10.1038/nature12187

## Cloning of Dirac fermions in graphene superlattices

L. A. Ponomarenko<sup>1</sup>, R. V. Gorbachev<sup>2</sup>, G. L. Yu<sup>1</sup>, D. C. Elias<sup>1</sup>, R. Jalil<sup>2</sup>, A. A. Patel<sup>1</sup>, A. Mishchenko<sup>1</sup>, A. S. Mayorov<sup>1</sup>, C. R. Woods<sup>1</sup>, J. R. Wallbank<sup>1</sup>, M. Mucha-Kruczynski<sup>1</sup>, B. A. Piot<sup>1</sup>, M. Potemski<sup>1</sup>, I. V. Grigorieva<sup>1</sup>, K. S. Novoselov<sup>1</sup>, F. Guinea<sup>1</sup>, V. I. Fal'ko<sup>3</sup> & A. K. Geim<sup>1,2</sup>

nature  
physics

ARTICLES

PUBLISHED ONLINE: 28 APRIL 2014 | DOI: 10.1038/NPHYS22954

## Commensurate-incommensurate transition in graphene on hexagonal boron nitride

C. R. Woods<sup>1</sup>, L. Britnell<sup>1</sup>, A. Eckmann<sup>2</sup>, R. S. Ma<sup>3</sup>, J. C. Lu<sup>3</sup>, H. M. Guo<sup>3</sup>, X. Lin<sup>3</sup>, G. L. Yu<sup>1</sup>, Y. Cao<sup>4</sup>, R. V. Gorbachev<sup>4</sup>, A. V. Kretinin<sup>1</sup>, J. Park<sup>1,5</sup>, L. A. Ponomarenko<sup>1</sup>, M. I. Katsnelson<sup>6</sup>, Yu. N. Gornostyrev<sup>7</sup>, K. Watanabe<sup>8</sup>, T. Taniguchi<sup>8</sup>, C. Casiraghi<sup>2</sup>, H.-J. Gao<sup>3</sup>, A. K. Geim<sup>4</sup> and K. S. Novoselov<sup>1\*</sup>

## Massive Dirac Fermions and Hofstadter Butterfly in a van der Waals Heterostructure

B. Hunt<sup>1,2\*</sup>, J. D. Sanchez-Yamagishi<sup>1,2\*</sup>, A. F. Young<sup>1,2\*</sup>, M. Yankowitz<sup>2</sup>, B. J. LeRoy<sup>2</sup>, K. Watanabe<sup>3</sup>, T. Taniguchi<sup>3</sup>, P. Moon<sup>4,†</sup>, M. Koshino<sup>4</sup>, P. Jarillo-Herrero<sup>1,†</sup>, R. C. Ashoori<sup>1,‡</sup>

LETTER

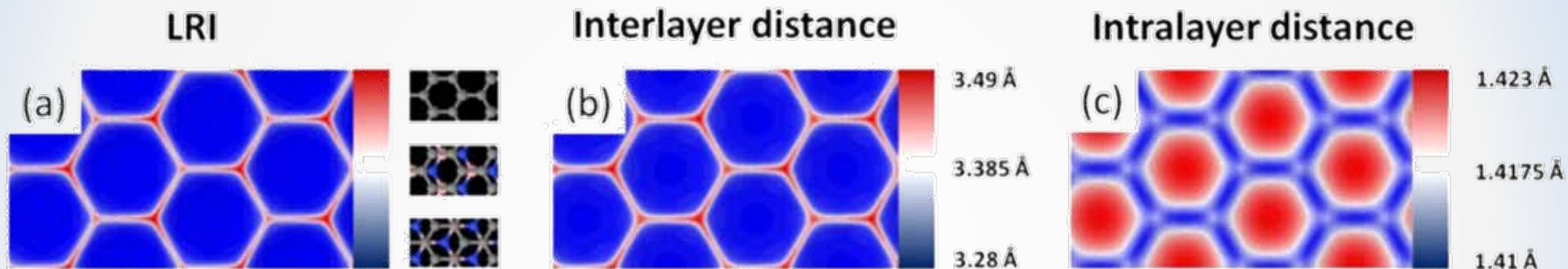
doi:10.1038/nature12186

## Hofstadter's butterfly and the fractal quantum Hall effect in moiré superlattices

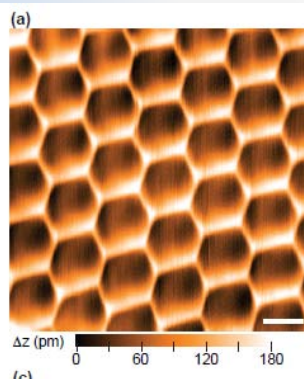
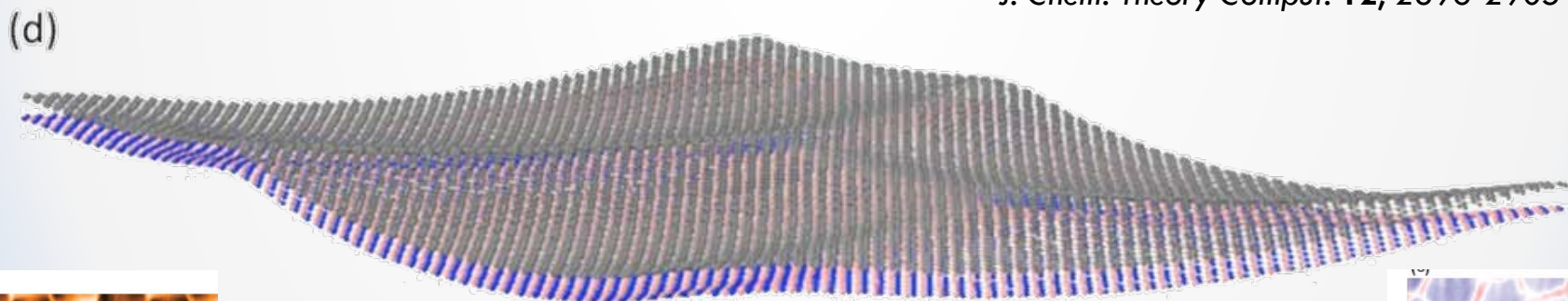
C. R. Dean<sup>1</sup>, L. Wang<sup>2</sup>, P. Maher<sup>3</sup>, C. Forsythe<sup>1</sup>, F. Ghahari<sup>3</sup>, Y. Gao<sup>2</sup>, J. Katoch<sup>4</sup>, M. Ishigami<sup>4</sup>, P. Moon<sup>5</sup>, M. Koshino<sup>5</sup>, T. Taniguchi<sup>6</sup>, K. Watanabe<sup>6</sup>, K. L. Shepard<sup>7</sup>, J. Hone<sup>8</sup> & P. Kim<sup>3</sup>

# Graphene/*h*-BN Hetero-Structures

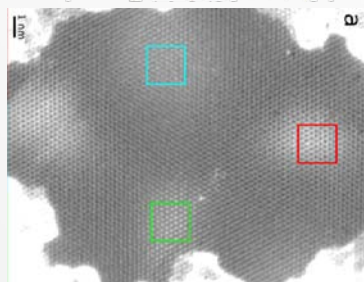
- Graphene and *h*-BN have an intralayer lattice mismatch of 1.83%.
- Moiré patterns result in domain walls.



*J. Chem. Theory Comput.* **12**, 2896-2905 (2016).

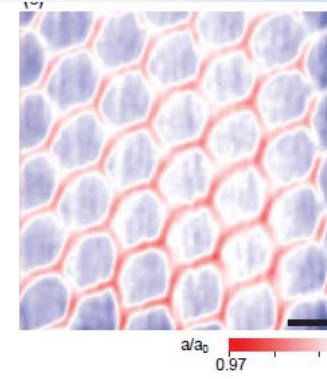


Surface corrugation



*Nano Lett.* **17**, 1409-1416 (2017)

Intra-layer bond lengths

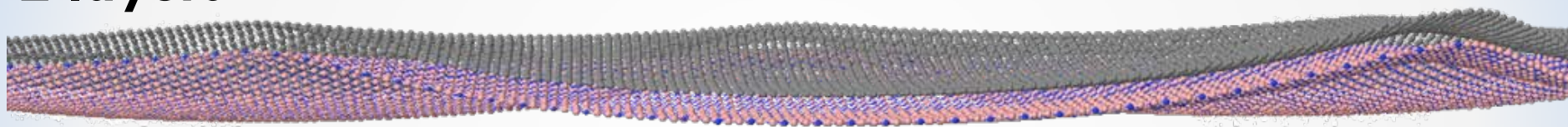


# Graphene/*h*-BN Hetero-Structures

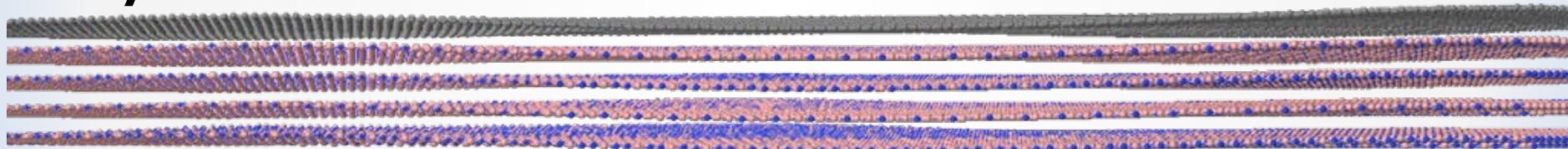
- The number of layers and interlayer misfit angle dictate the relaxed structure.

**2 layers**

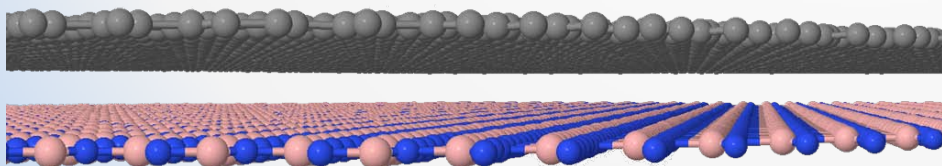
**0° Misfit angle**



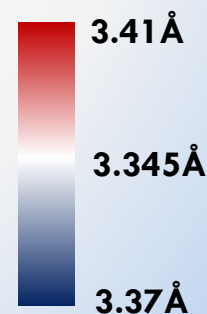
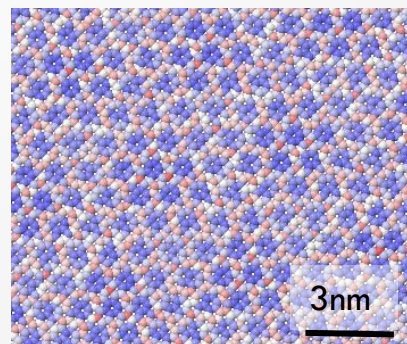
**5 layers**



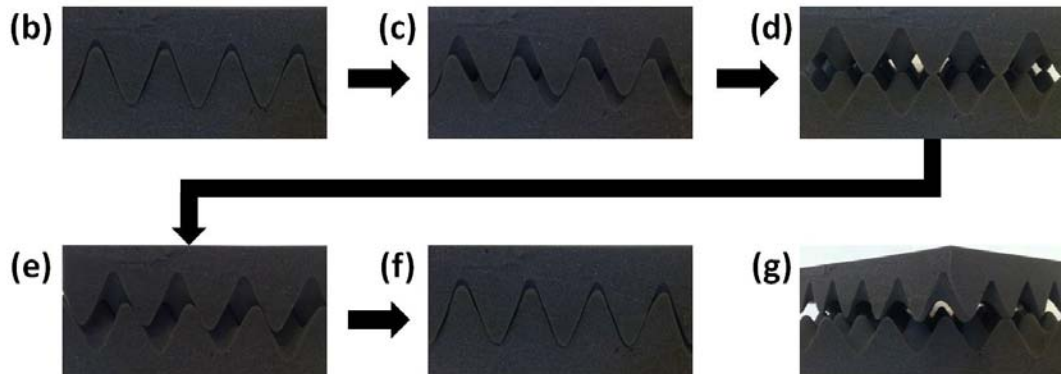
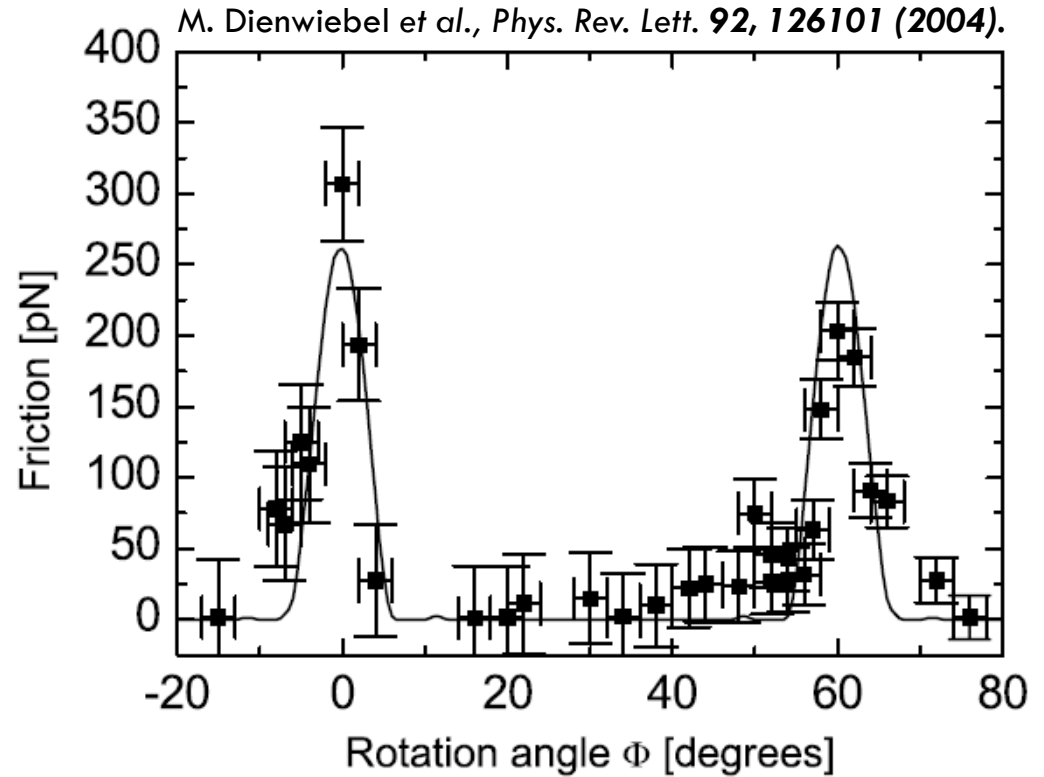
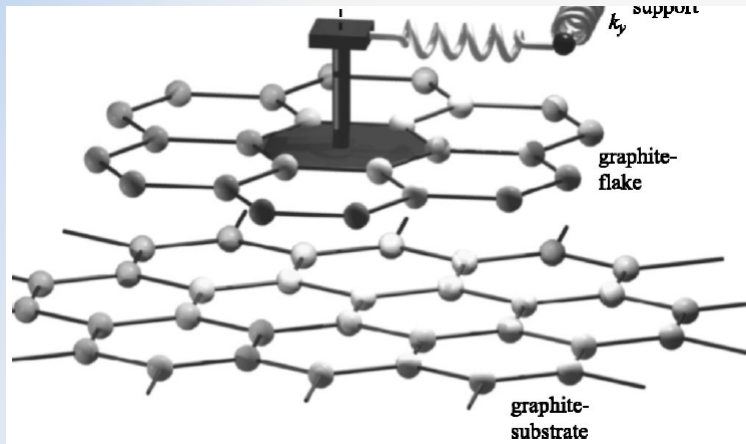
**20° Misfit angle, bilayer**



corrugation  $\sim 0.03\text{\AA}$



# Robust Superlubricity in Heterojunctions



Can nanoscale graphitic interfaces exhibit sustainable superlubric behavior?

# Robust Superlubricity in Heterojunctions

PRL **100**, 046102 (2008)

PHYSICAL REVIEW LETTERS

week ending  
1 FEBRUARY 2008

## Torque and Twist against Superlubricity

Alexander E. Filippov,<sup>1</sup> Martin Dienwiebel,<sup>2,3</sup> Joost W. M. Frenken,<sup>2</sup> Joseph Klafter,<sup>4</sup> and Michael Urbakh<sup>4</sup>

Nanoscale graphene flakes dynamically rotate and lock in the commensurate high friction state.

THE JOURNAL OF  
PHYSICAL CHEMISTRY  
*Letters*

Letter

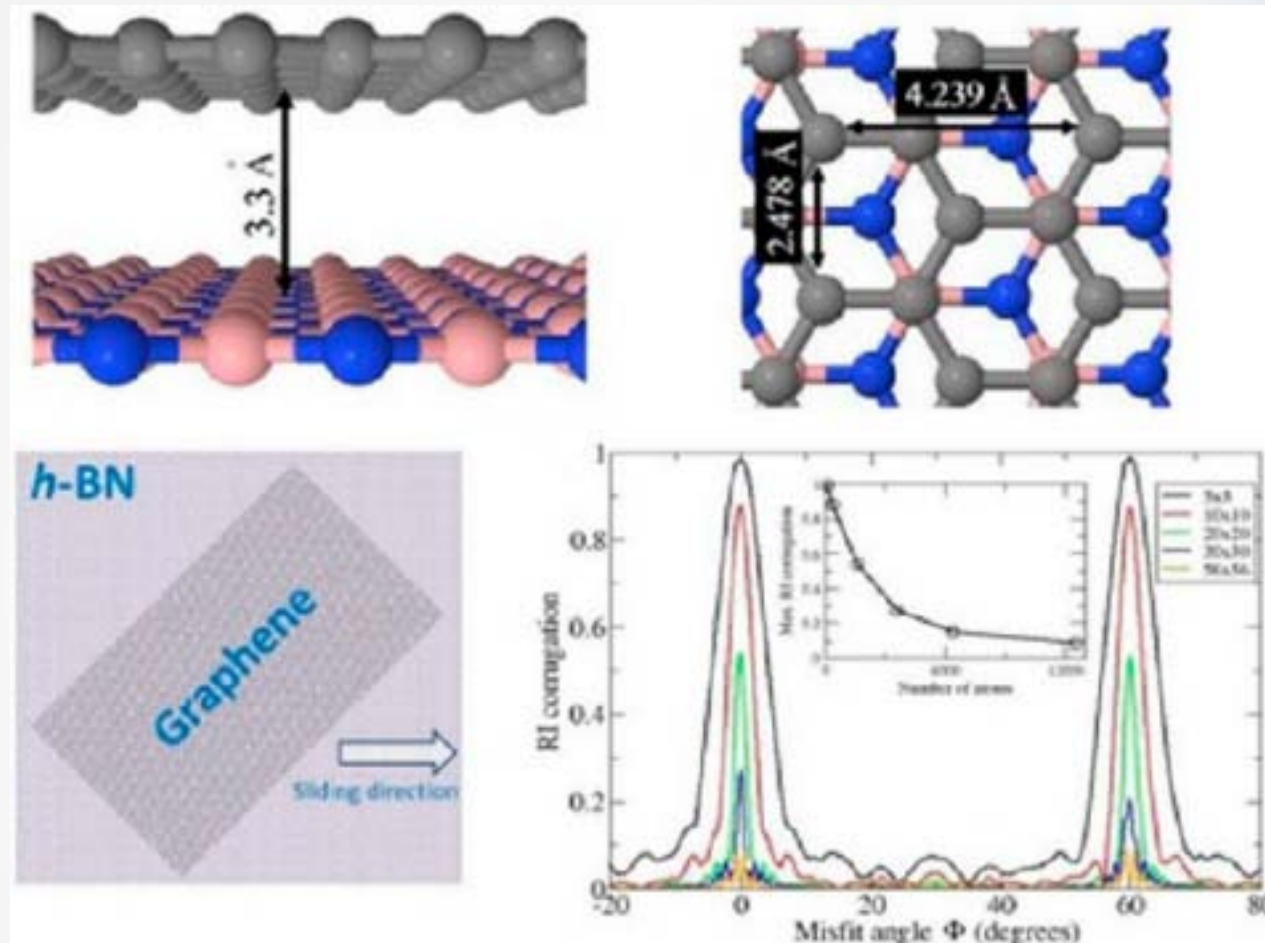
[pubs.acs.org/JPCL](http://pubs.acs.org/JPCL)

## Robust Superlubricity in Graphene/*h*-BN Heterojunctions

Itai Leven, Dana Krepel, Ortal Shemesh, and Oded Hod\*

Due to the intrinsic 1.8% lattice vector mismatch of the hexagonal lattices of graphene and *h*-BN their heterogeneous junction is expected to present superlubric behavior regardless of their relative orientation.

# Robust Superlubricity in Heterojunctions



- Geometric modeling of rigid surfaces using the Registry Index method demonstrated that for large enough flakes robust superlubricity can be achieved by considerably reducing the PES (and hence friction) anisotropy.
- Neglecting dynamic effects!



# Robust Superlubricity in Heterojunctions

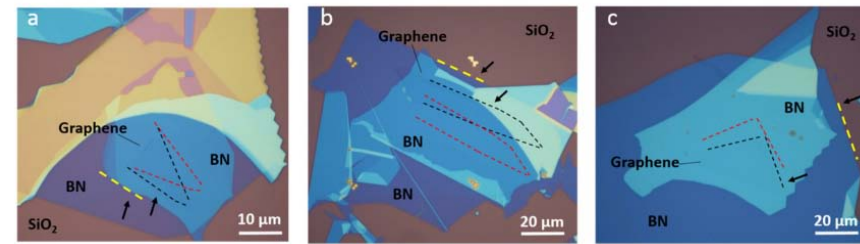
## Self orientation of graphene sandwiched between *h*-BN surfaces.

Evidence for a fractional fractal quantum Hall effect in graphene superlattices

Lei Wang<sup>1,2</sup>, Yuanda Gao<sup>1</sup>, Bo Wen<sup>3</sup>, Zheng Han<sup>3</sup>, Takashi Taniguchi<sup>4</sup>, Kenji Watanabe<sup>4</sup>, Mikito Koshino<sup>5</sup>, James Hone<sup>1</sup>, ...

+ See all authors and affiliations

Science 04 Dec 2015;  
Vol. 350, Issue 6265, pp. 1231-1234  
DOI: 10.1126/science.aad2102



## Self orientation of graphene on *h*-BN.



Altmetric: 4 Views: 4,123 Citations: 6 More detail >>

Article | OPEN

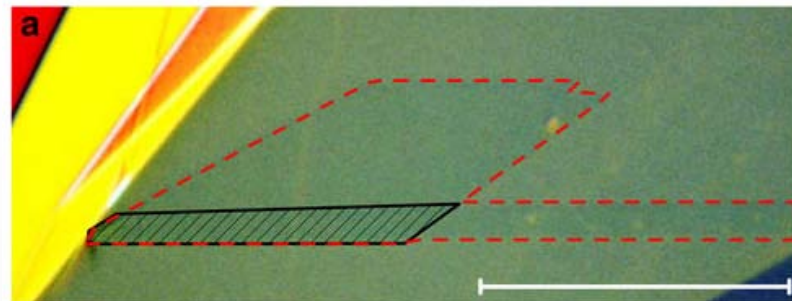
## Macroscopic self-reorientation of interacting two-dimensional crystals

C. R. Woods, F. Withers, M. J. Zhu, Y. Cao, G. Yu, A. Kozikov, M. Ben Shalom, S. V. Morozov, M. M. van

Wijk, A. Fasolino, M. I. Katsnelson, K. Watanabe, T. Taniguchi, A. K. Geim, A. Mishchenko & K. S.

Novoselov

Figure 1: Optical and atomic force microscopy of a self-rotating flake.



## Multi-contact superlubricity in graphene/graphene and graphene/*h*-BN junctions.

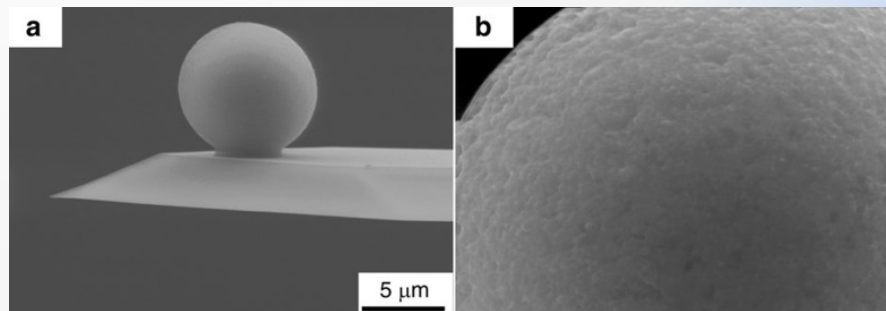


Nat Commun 2017; 8: 14029.  
Published online 2017 Feb 14. doi: 10.1038/ncomms14029

PMCID: PMC5316838

## Robust microscale superlubricity under high contact pressure enabled by graphene-coated microsphere

Shu-Wei Liu,<sup>1</sup> Hua-Ping Wang,<sup>2</sup> Qiang Xu,<sup>3</sup> Tian-Bao Ma,<sup>a,1</sup> Gui Yu,<sup>b,2</sup> Chenhui Zhang,<sup>1</sup> Dechao Geng,<sup>2</sup> Zhiwei Yu,<sup>1</sup> Shengguang Zhang,<sup>3</sup> Wenzhong Wang,<sup>3</sup> Yuan-Zhong Hu,<sup>1</sup> Hui Wang,<sup>1</sup> and Jianbin Luo<sup>c,1</sup>



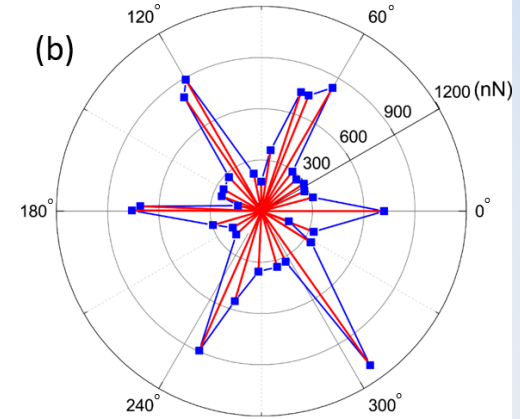
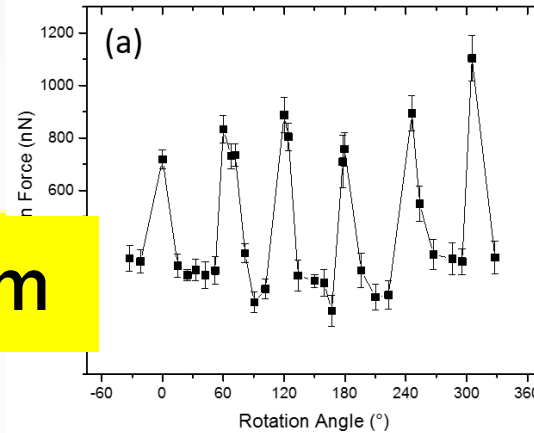
# Robust Superlubricity in Heterojunctions

Robust superlubricity in microscale graphene/*h*-BN heterostructures

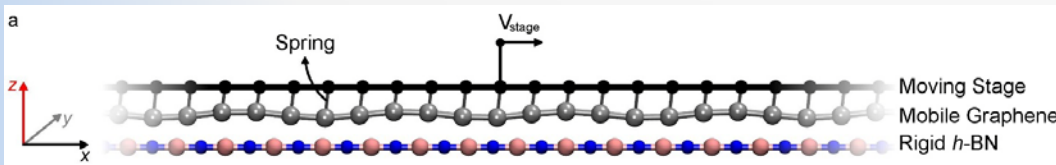
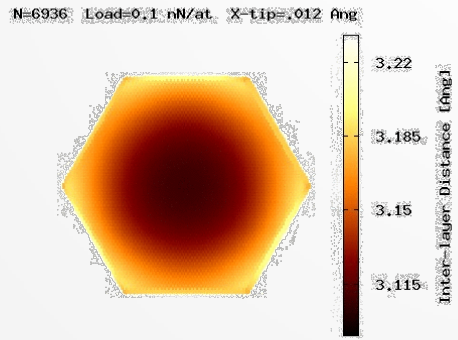
(i) (ii)

Weak anisotropy

Different Mechanism



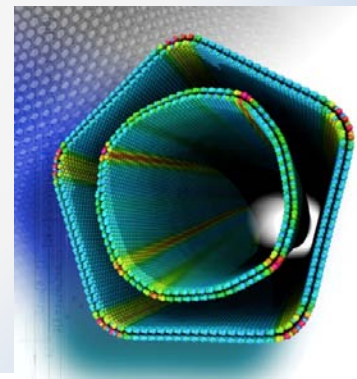
Some cool fully atomistic molecular dynamics simulations



Davide Mandelli  
Tomorrow @ 14:20

# Classical Force-Fields Applications

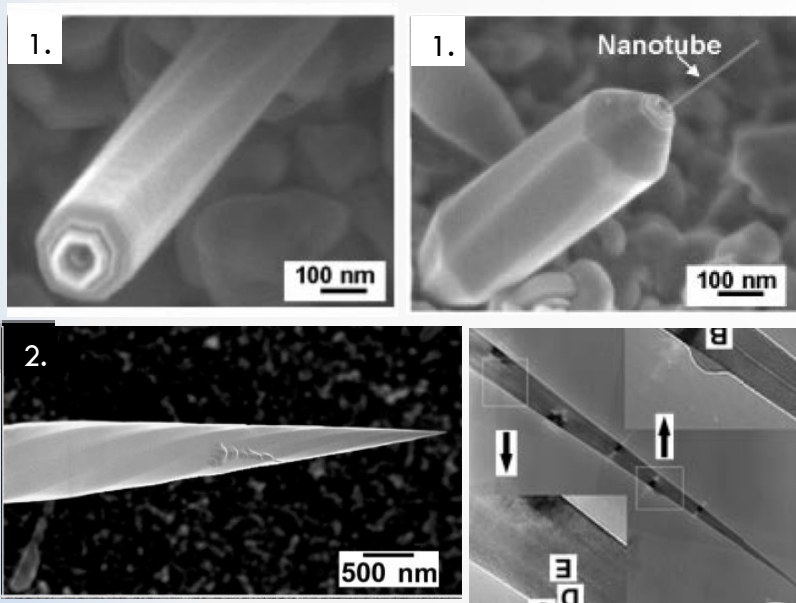
## Nanotube Faceting



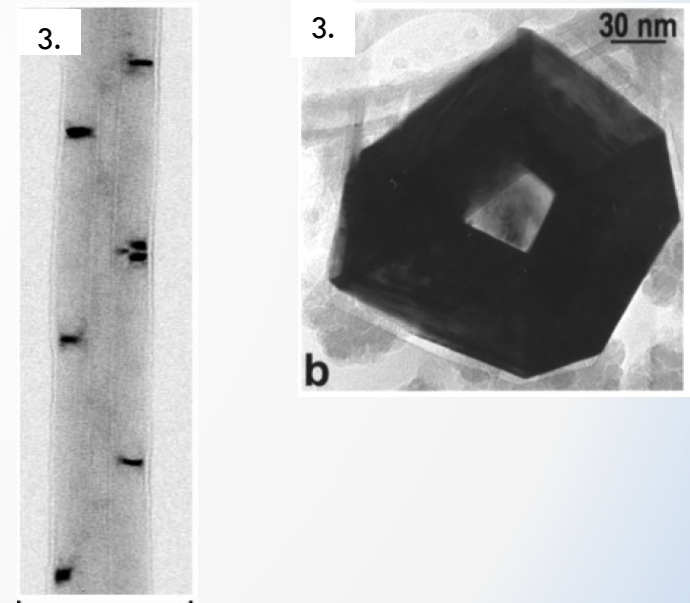
# Faceting in Multi-Walled Nanotubes

- Nanotubes are often considered to have cylindrical cross sections.
- MWNTs can exhibit circumferential faceting.
- Faceting is more abundant in MWBNNTs than in MWCNTs.

## Carbon



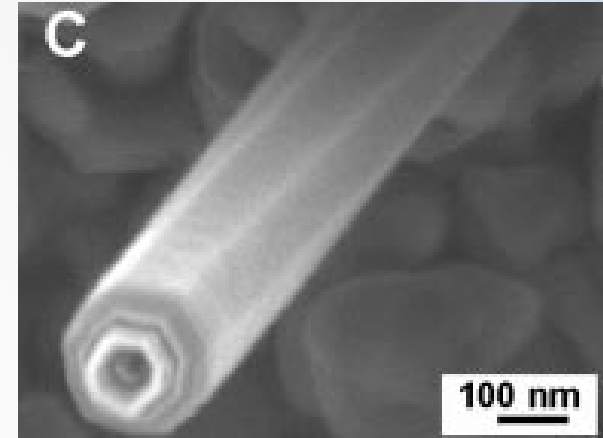
## BN



1. G. Zhang, X. Jiang, E. Wang, *Science* **300**, 472 (2003).
2. Y. Gogotsi, J. A. Libera, N. Kalashnikov, M. Yoshimura, *Science* **290**, 317 (2000).
3. A. Celik-Aktas, J. Zuo, J. F. Stubbins, C. Tang and Y. Bando, *Acta Cryst.* (2005). A61, 533.

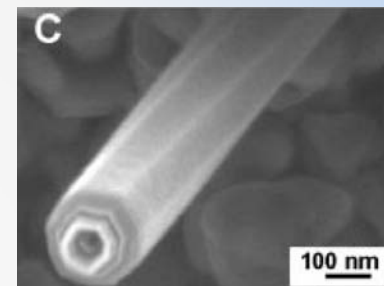
# Faceting in Multi-Walled Nanotubes

- Open questions:
  - ✓ Why do facets form?
  - ✓ What dictates the number of facets?
  - ✓ What determines the facet helicity?
  - ✓ Why are facets more abundant in MWBNNTs than in MWCNTs?
  - ✓ How does faceting influence the mechanical and tribological properties of MWNTs?



# Nanotube Faceting and Local Registry

Science, 290, 317 (2000)



- The anisotropic interlayer potential of Kolmogorov and Crespi (*Phys. Rev. B* **71**, 235415 (2005)) for graphitic systems and our *h*-BN-ILP (*J. Chem. Phys.* **140**, 104106 (2014)) are used to perform geometry optimizations of double walled nanotubes.

I. Leven, R. Guerra, A. Vanossi, E. Tosatti, and O. Hod, "Multi-Walled Nanotube Faceting Unravalled", *Nat. Nanotechnol.* **11**, 1082-1086 (2016).

✓ ZZ@ZZ and AC@AC DWNTs form facets.

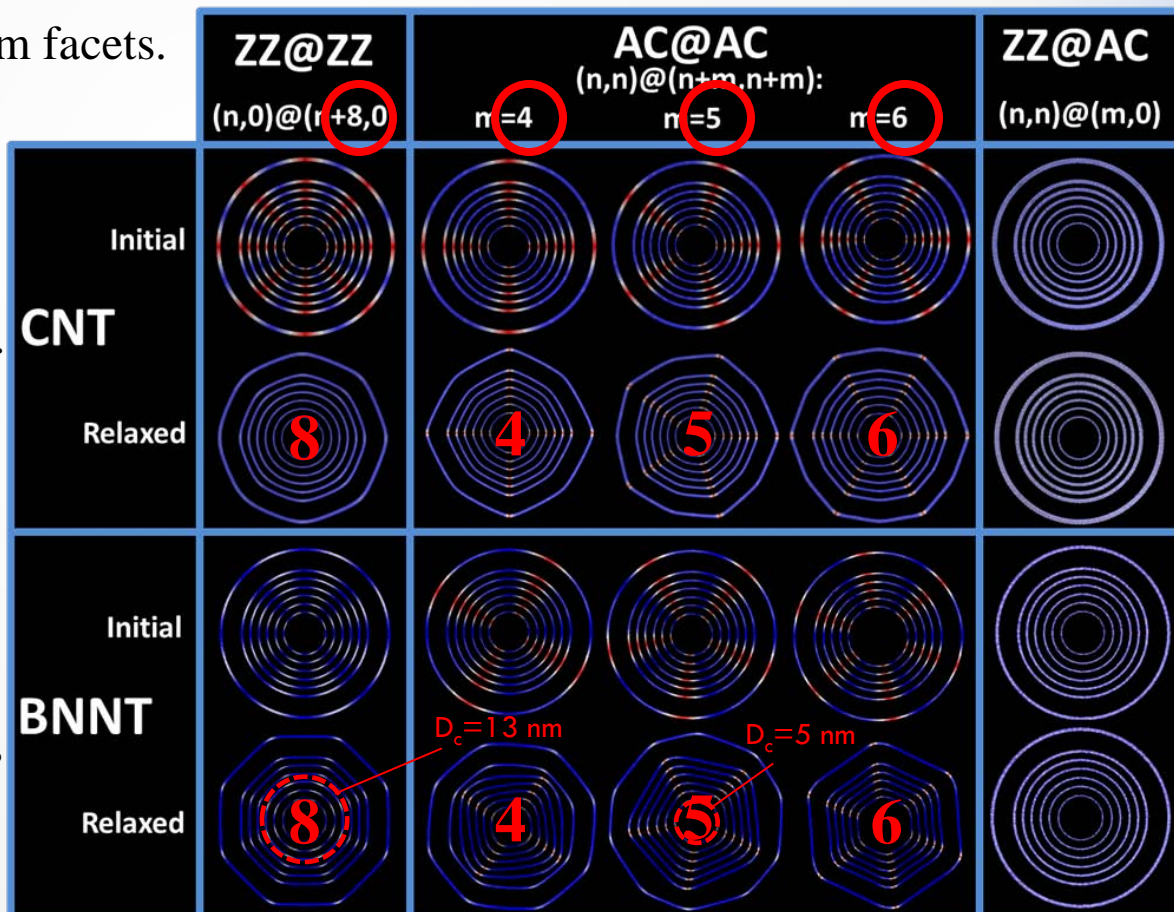
✓ ZZ@AC do not facet.

✓ The critical diameter for faceting is 5-13 nm in agreement with experiment (*Nano Lett.* **12**, 6347-6352 (2012)).

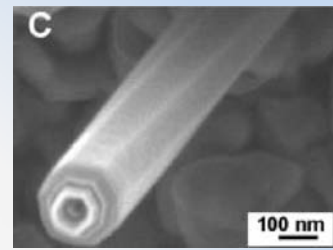
✓ Number of facets equals the difference in the number of circumferential unit cells.

✓ Local registry patterns reveal that the difference in circumferential unit cells distributes evenly around the nanotube.

✓ Bad registry regions form vertices.



# Chiral DWNT Nanotube Faceting



Science, 290, 317 (2000)

- Local registry patterns determine faceting in chiral DWNTs, as well.
- Mono-chiral DWNTs form non-uniform axial patterns.
- Bi-chiral DWNTs form spiraling facets. Their helical angle grows with the chiral angle difference and their length reduces.
- The interlayer spacing is close to equilibrium at the facets and increases at the vertices.

$\Delta\theta=0^\circ$

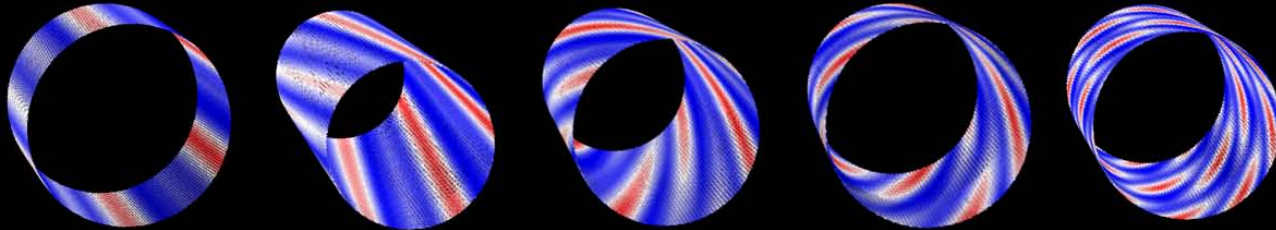
$\Delta\theta=0.252^\circ$

$\Delta\theta=0.657^\circ$

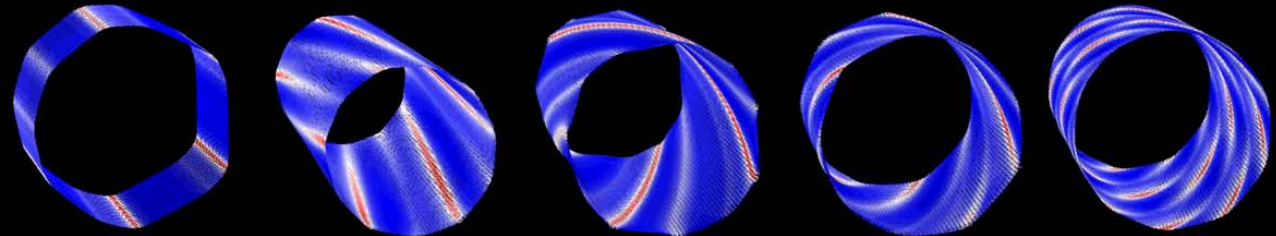
$\Delta\theta=1.14^\circ$

$\Delta\theta=1.74^\circ$

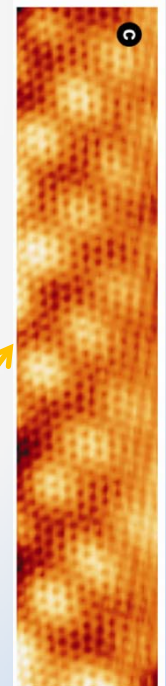
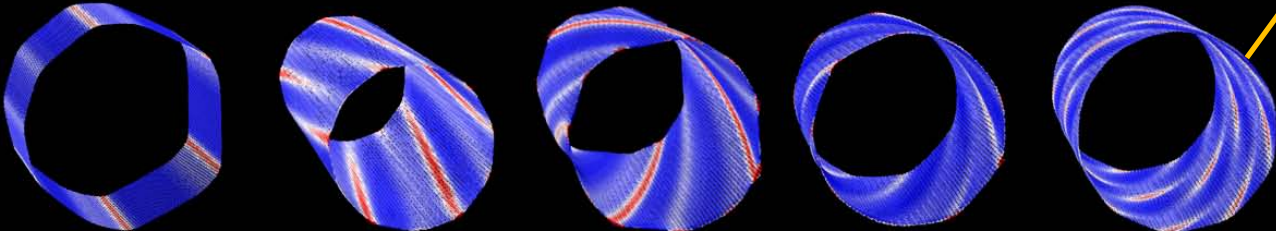
LRI  
Initial:



LRI  
Relaxed:



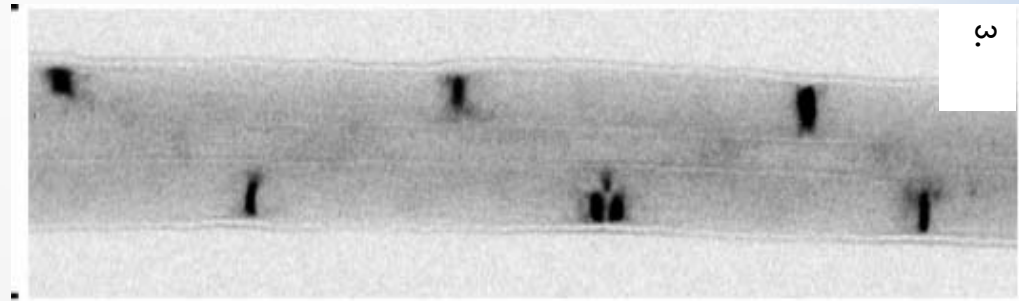
IL spacing  
Relaxed:



Carbon 61, 379 (2013)

# Why is faceting more abundant in BNNTs than in CNTs?

- Faceting requires chiral angle matching between adjacent layer.
- MWBNNTs present high uniformity in the chirality of the different layers whereas MWCNTs have a much wider distribution of wall chiralities.
- This is a result of the larger interlayer adhesion in *h*-BN and the weak, yet important (when summed over large surfaces), electrostatic interactions between the partially charged atomic centers in BNNT that is absent in CNTs.





# Classical Force-Fields Applications

## Nanotube Friction

# Enhance Friction in MWBNNTs

LETTERS

PUBLISHED ONLINE: 1 JUNE 2014 | DOI: 10.1038/NMAT3985

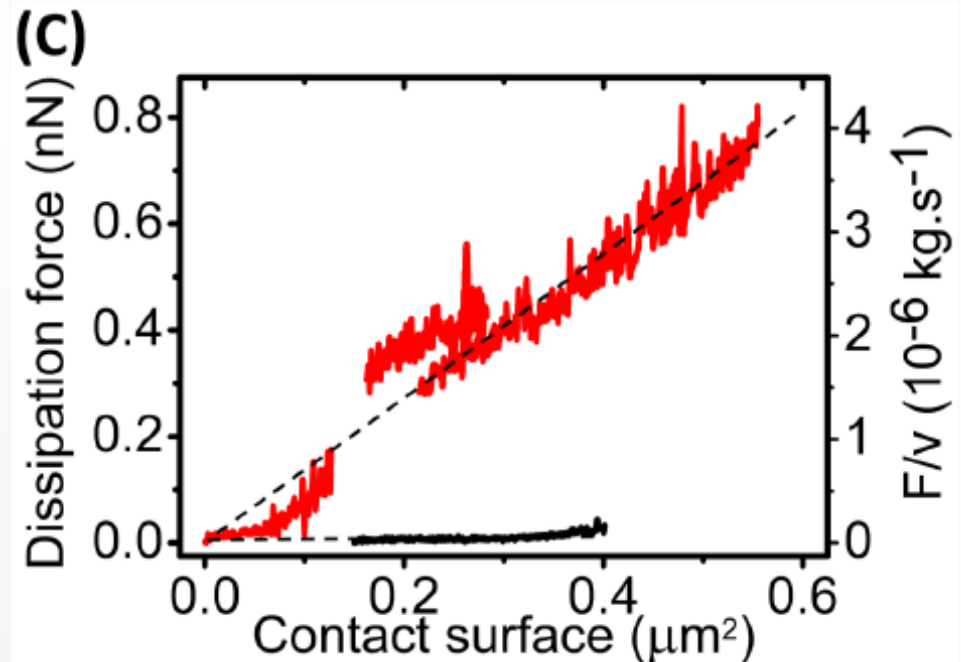
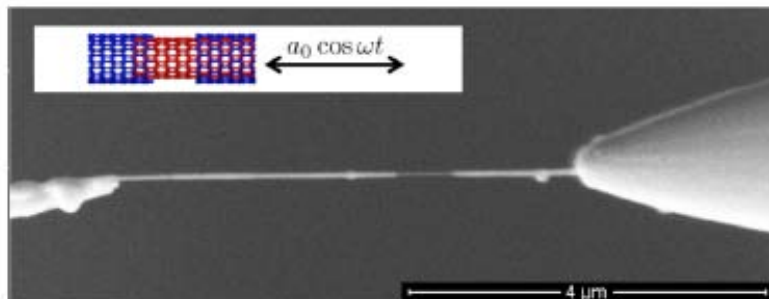
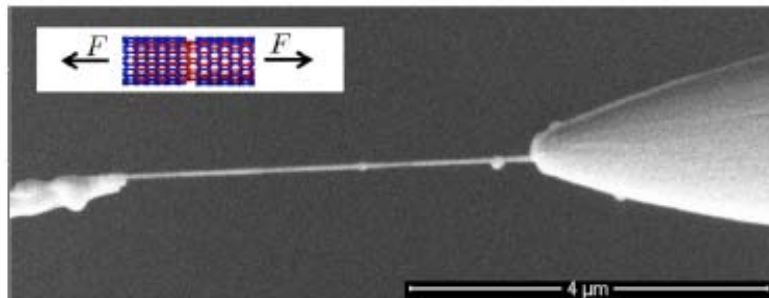
nature  
materials

## Ultrahigh interlayer friction in multiwalled boron nitride nanotubes

A. Niguès<sup>1</sup>, A. Siria<sup>1\*</sup>, P. Vincent<sup>1</sup>, P. Poncharal<sup>1</sup> and L. Bocquet<sup>1,2</sup>

688

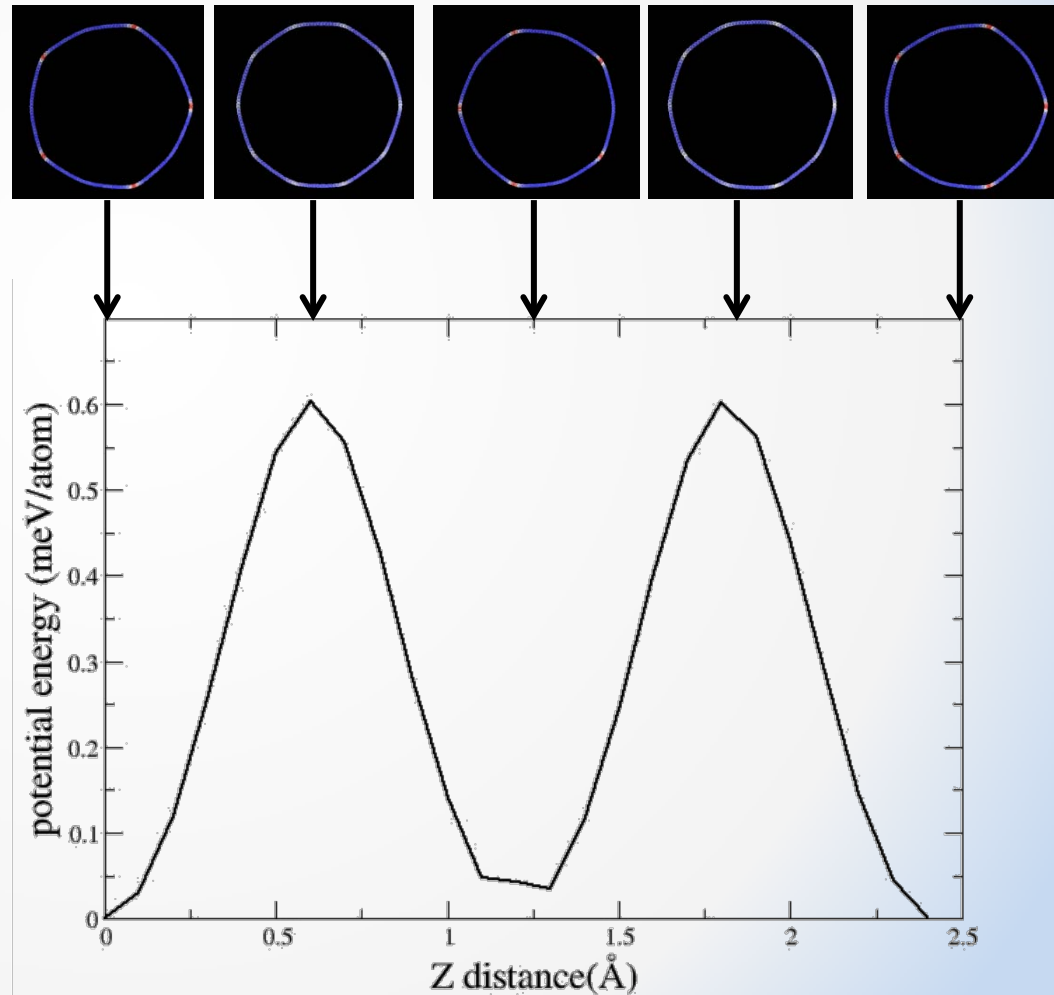
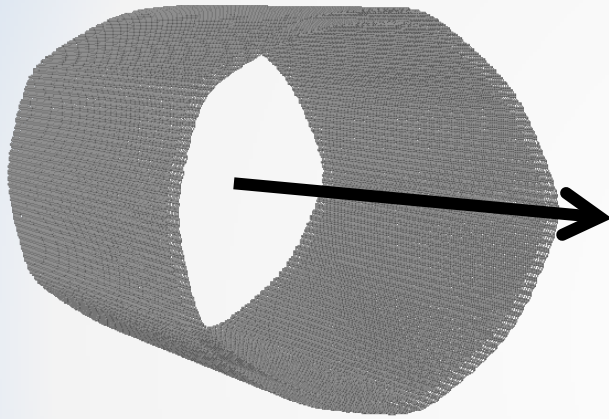
NATURE MATERIALS | VOL 13 | JULY 2014 | [www.nature.com/naturematerials](http://www.nature.com/naturematerials)



# Facet Superstructure Reconfiguration

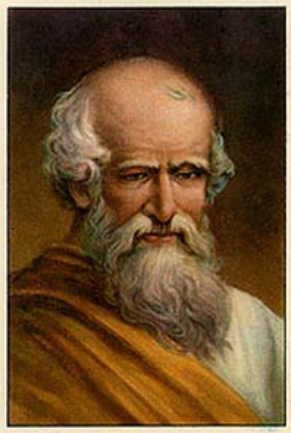
- Inter-wall pullout can cause facet superstructure reconfiguration

AC (75,75)@(80,80) DWCNT



# Facet Superstructure Reconfiguration

## Telescopic motion of bi-chiral DWBNNT



FRONT VIEW

PERSPECTIVE VIEW

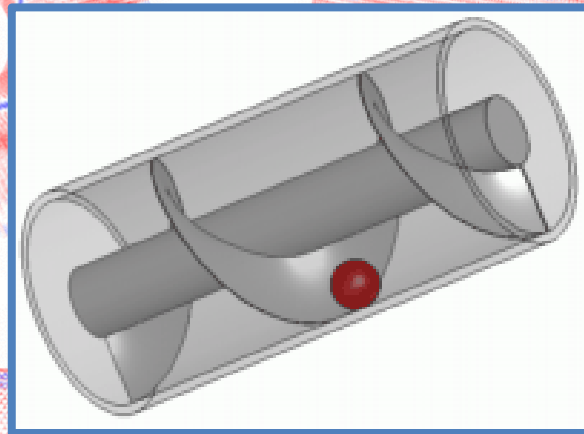
Bi-chiral DWBNNT (70,70)@(77,74)

$\Delta\theta = 0.76$  deg

interlayer energy:

low E

SIDE VIEW



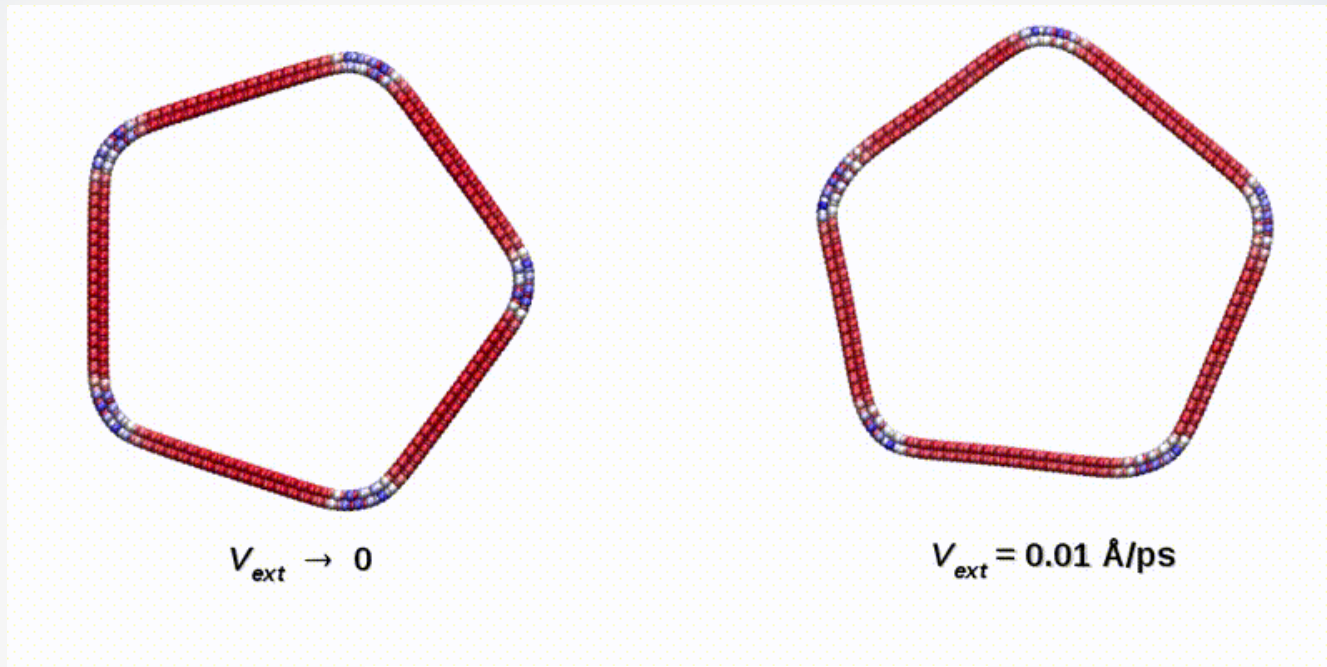
**Archimedean screw**

Internal (external) tube  
c.o.m. velocity is fixed  
at  $v_{\text{ext}}(0)$ .



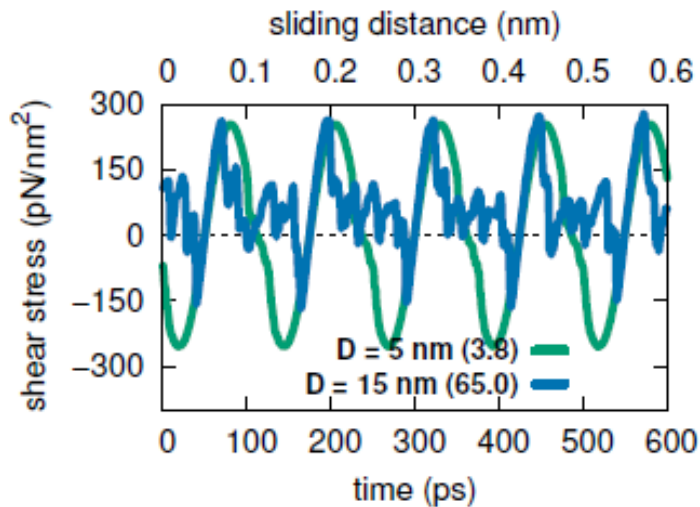
PBC along tube axis

# Faceting Induced Friction

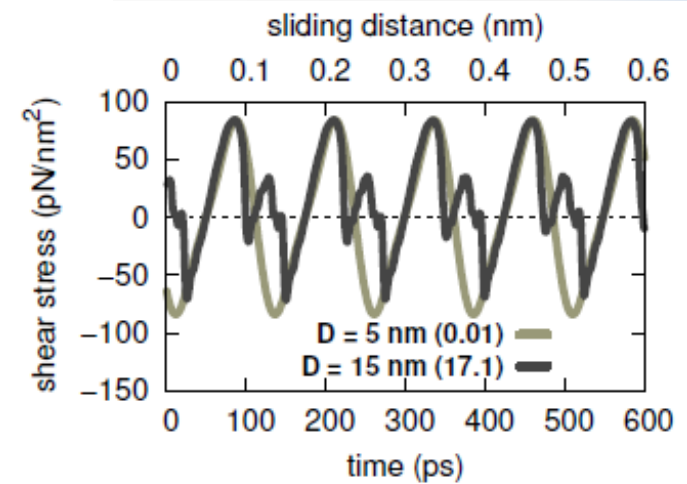


Armchair

DWBNNTs

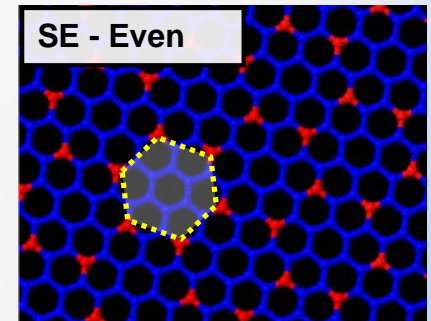
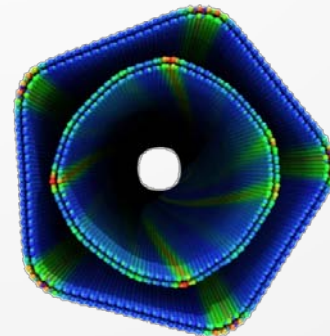
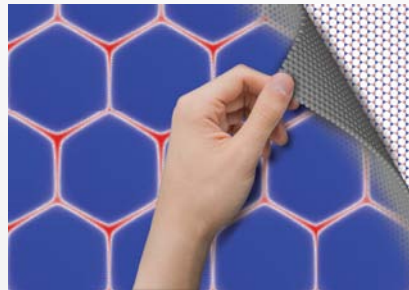
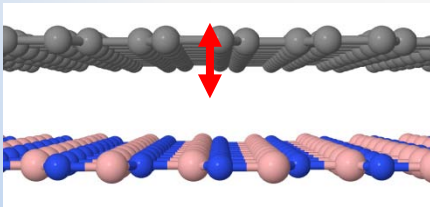


DWCNTs



# Conclusions

- ✓ Dedicated inter-layer force-fields have been developed for *h*-BN and graphene/*h*-BN.
- ✓ Inter-layer registry patterns dictate the super-structure of domain-wall formation in graphene/*h*-BN and faceting in multi-walled nanotubes.
- ✓ These are manifested in their tribological characteristics.
- ✓ Cross-layer transport is also highly dependent on the inter-layer registry.
- ✓ The force-field is transferable to other 2D materials.



# Acknowledgements

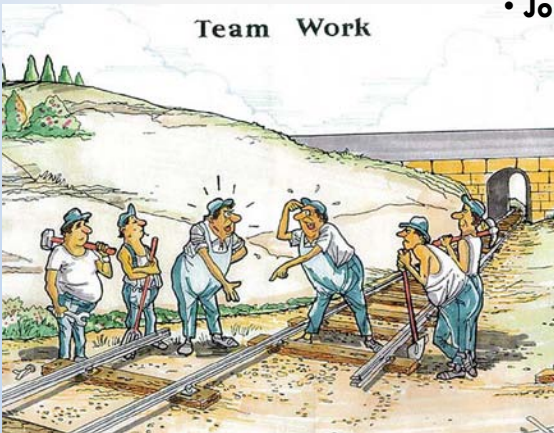
- Leeor Kronik
- Alexandre Tkatchenko
- Michael Urbakh
- Ernesto Joselevich
- Urs T. Dürig
- Erio Tosatti

- Itai Leven
- Inbal Oz
- Tal Maaravi
- Ido Azuri
- Davide Mandelli
- Noa Marom
- Jonathan Garel
- Elad Koren
- Roberto Guerra
- Andrea Vanossi
- Yaron Itkin
- Lena Kalikhman-Razvozov
- Inbal Zaltsman
- Adi Blumberg
- Uri Keshet
- Asaf Buchwalter
- Katherine Akulov
- Jonny Bernstein

- ISF 1313/08.
- TAU Nanocenter.
- MOD.



- The Lise-Meitner – Minerva Center for computational chemistry.
- The Raymond and Beverly Sackler Center for Computational Molecular and Materials Science.



And you  
For your attention!