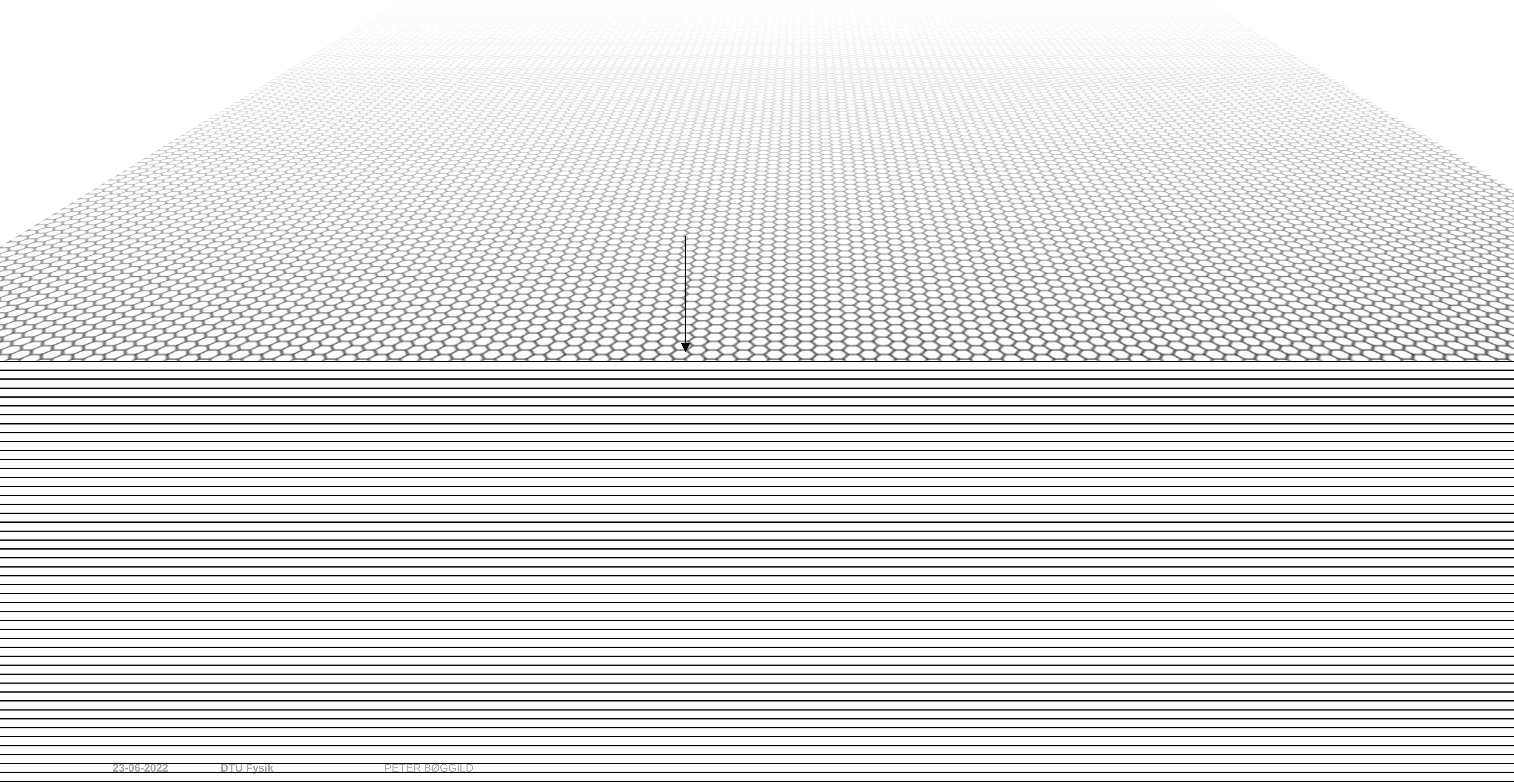
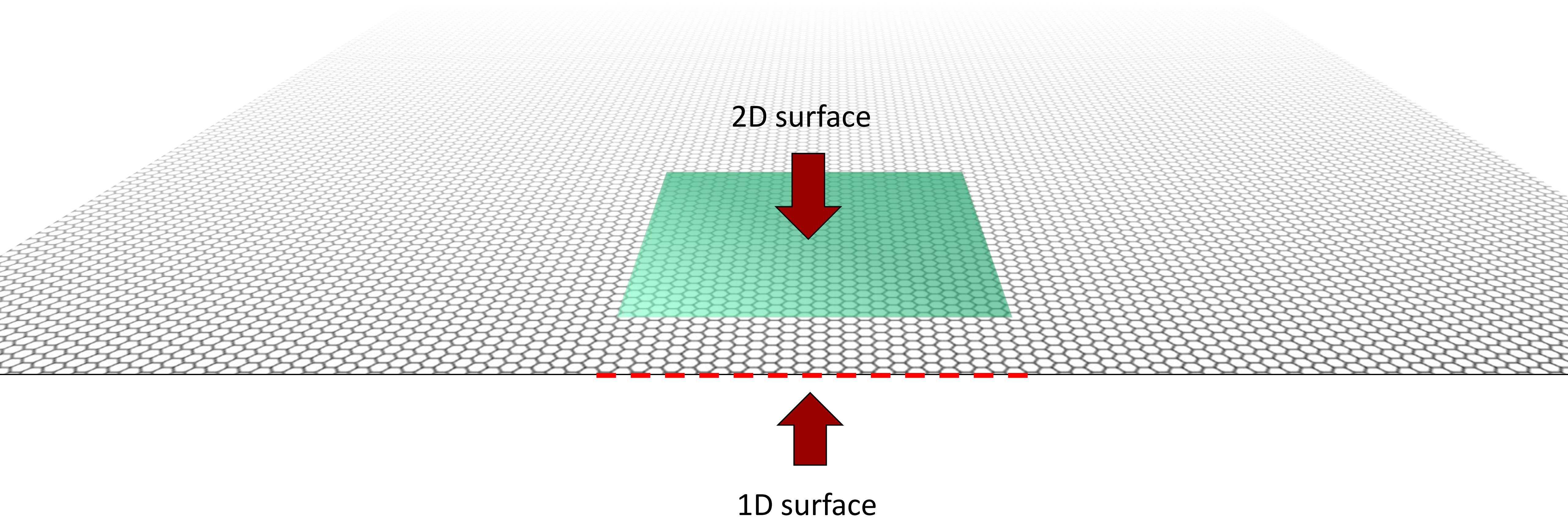
Van der Waals epitaxy

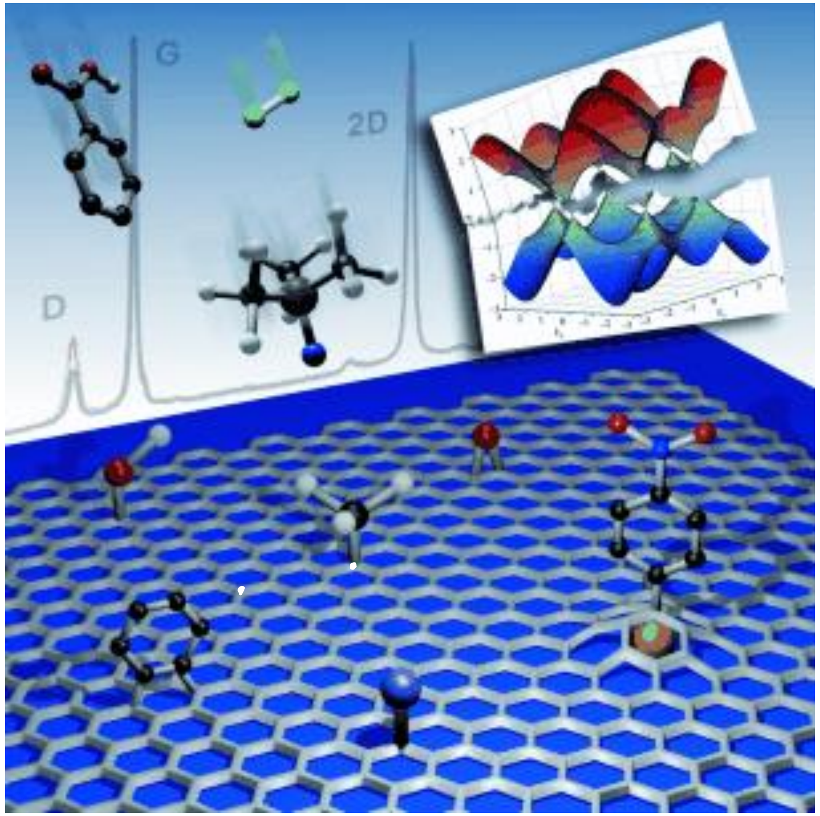
Peter Bøggild, Physics Department, Technical University of Denmark



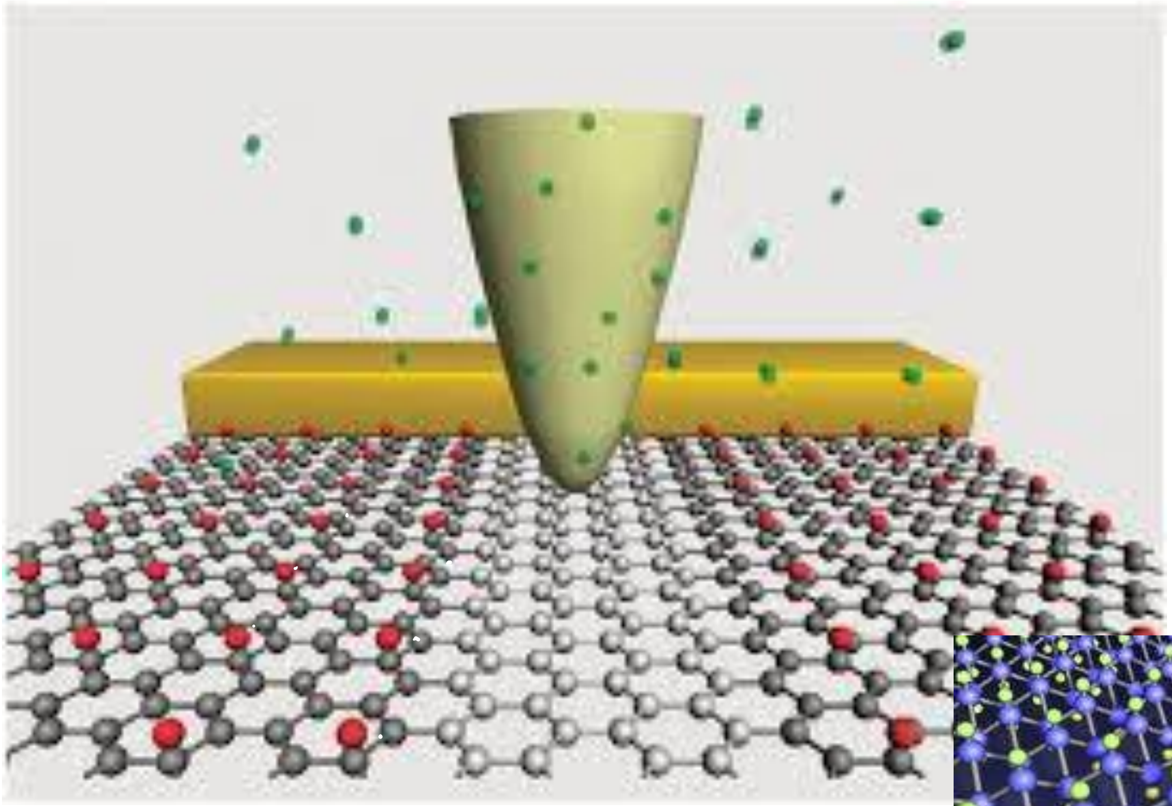


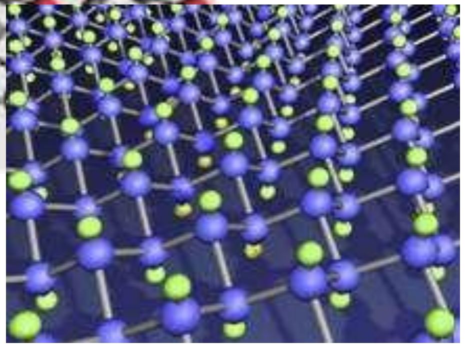
In a 2D material the bulk is a surface, and the surface is an edge

Functionalise 2D material with other molecules

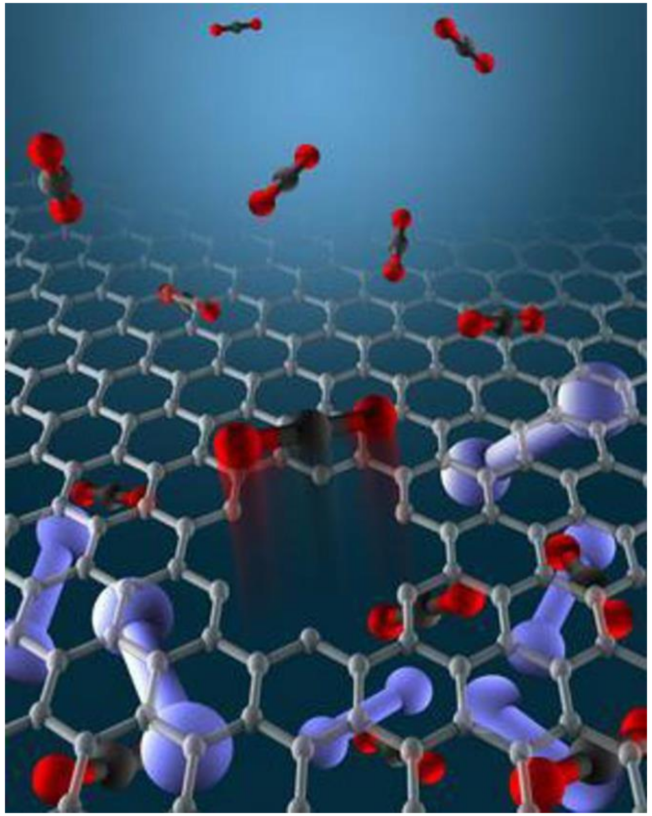


Convert 2D material into another material, and back



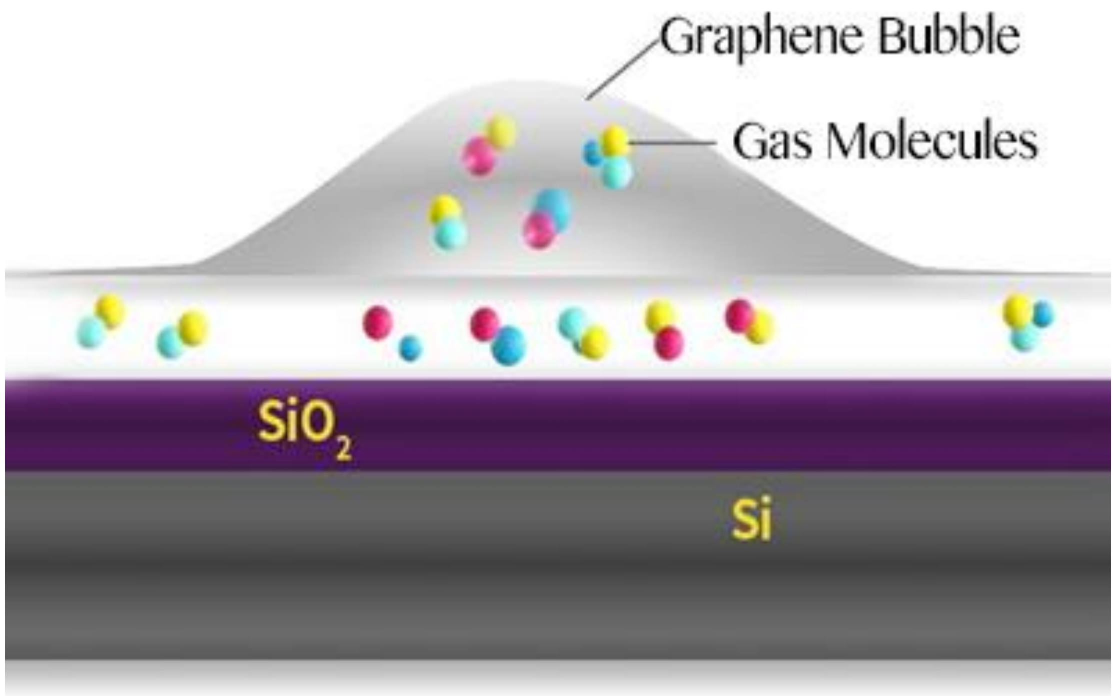


Create holes for ionfilters, molecular sieves, and DNA translocation



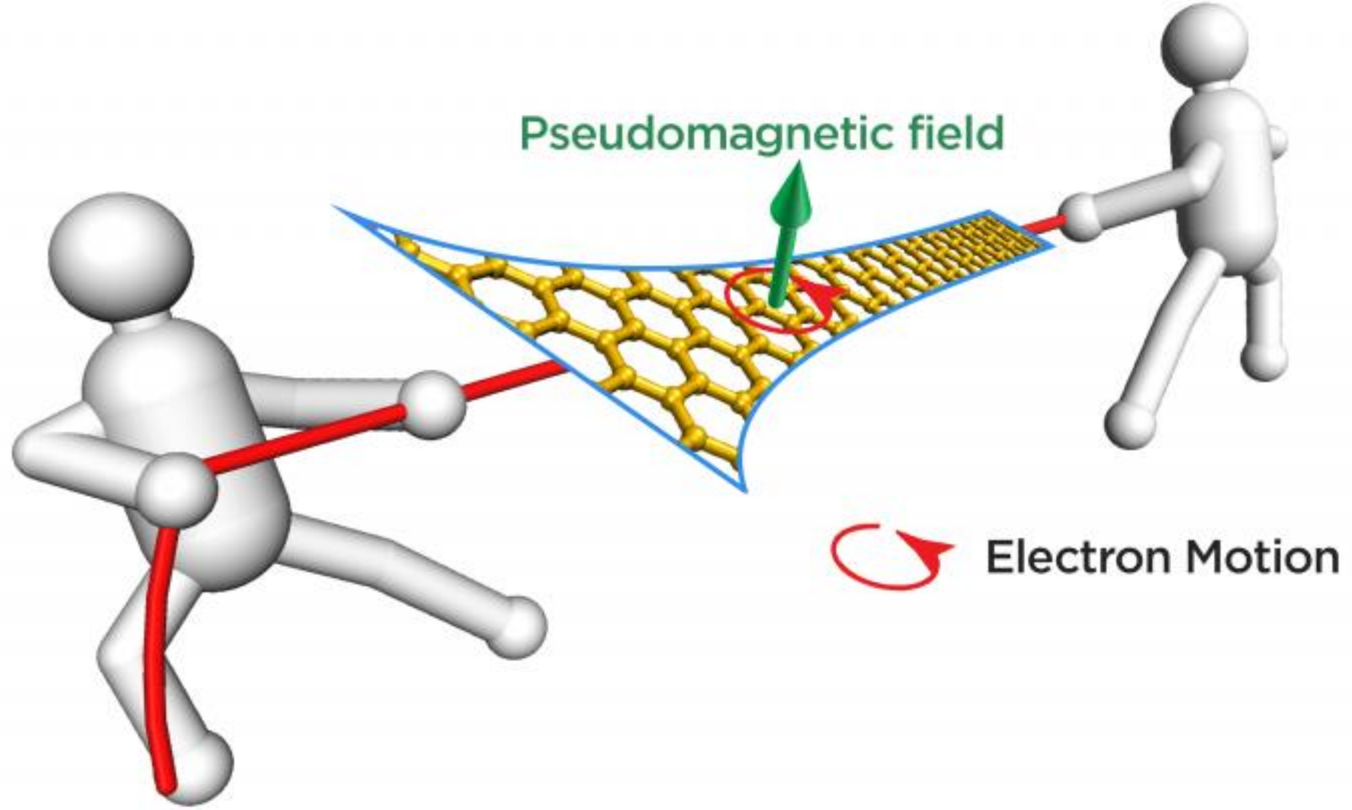
https://spectrum.ieee.org/graphenebased-gas-membranes-promise-reduced-carbon-dioxide-emissions

Trap molecules and do chemical reactions inside attoliter cavities, with extreme reaction rates

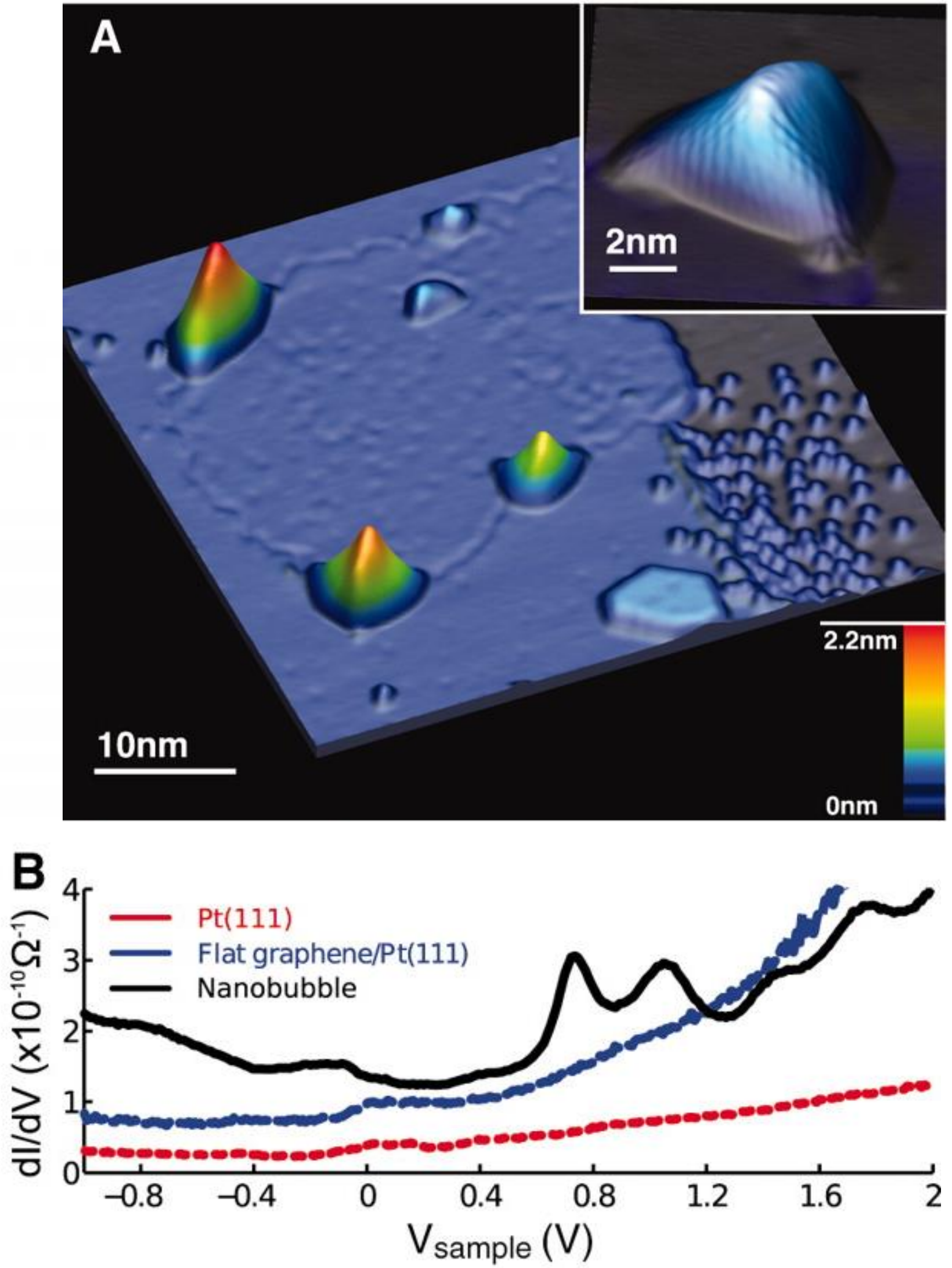


- Yuan Huang, Xiao Wang, Xu Zhang, Xianjue Chen, Baowen Li, Bin Wang, Ming Huang, Chongyang Zhu, Xuewei Zhang, Wolfgang S. Bacsa, Feng Ding, and Rodney S. Ruoff; "Raman Spectral Band Oscillations in Large Graphene Bubbles"; Phys. Rev. Lett.; 2018

Create strong pseudomagnetic fields by straining graphene

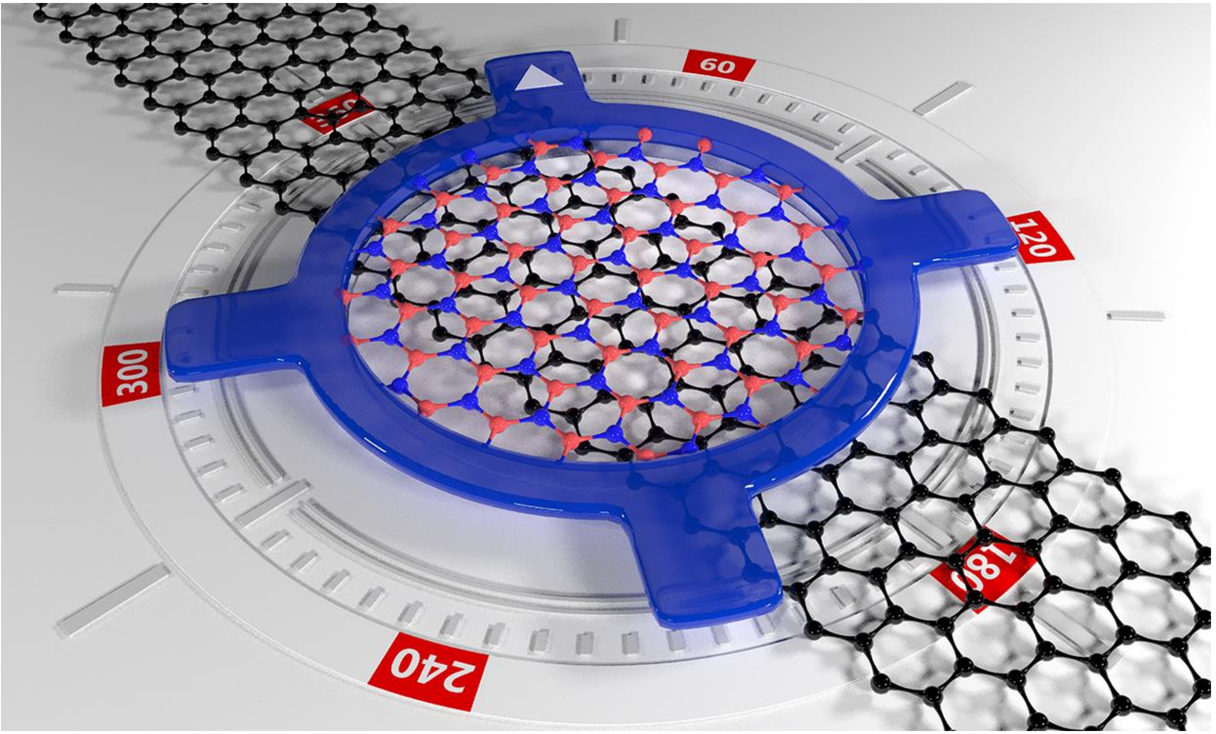


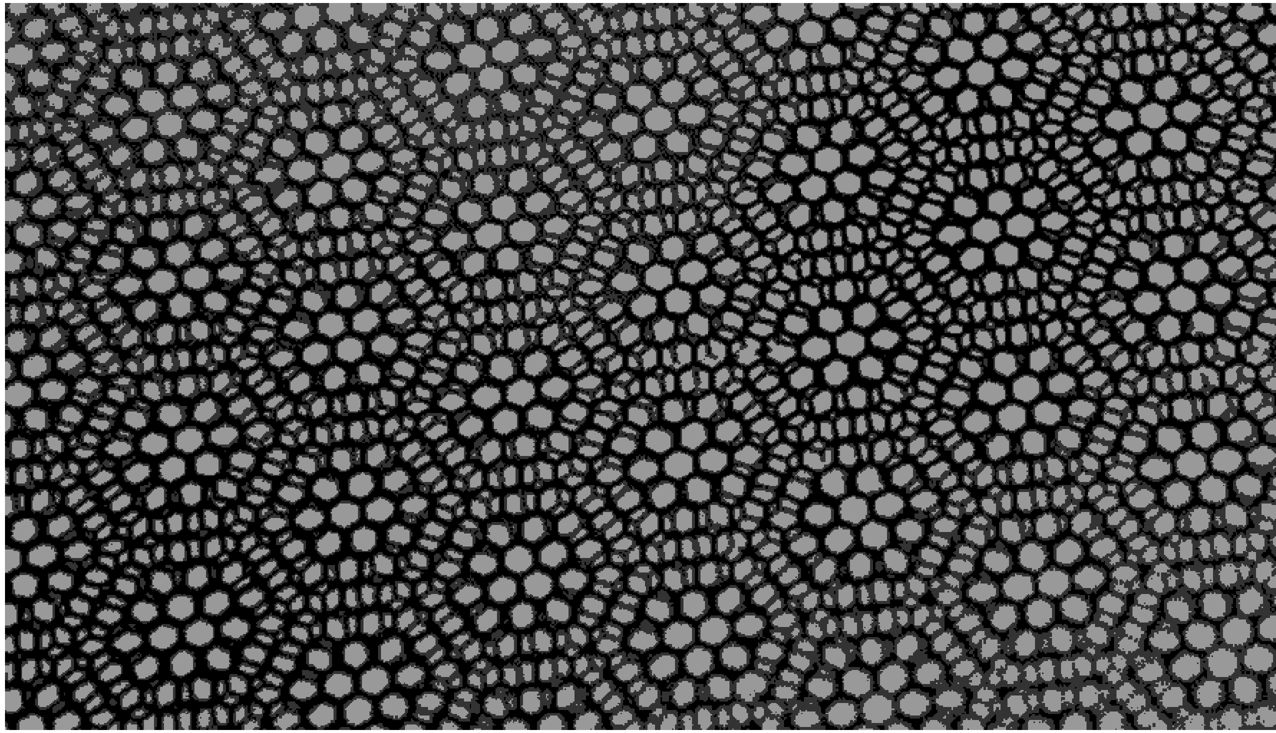
PRL 115, 245501 (2015)



30 JULY 2010 VOL 329 SCIENCE www.sciencemag.org

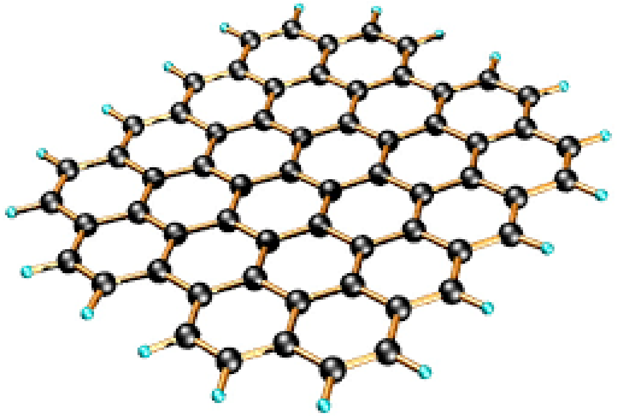
Create new electronic or photonic properties by controlling twist angle between two crystals





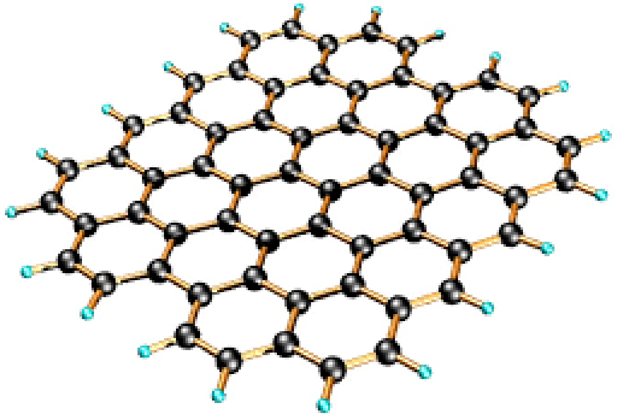
https://spectrum.ieee.org/a-twist-in-graphene-could-make-for-tunable-electronic-devices

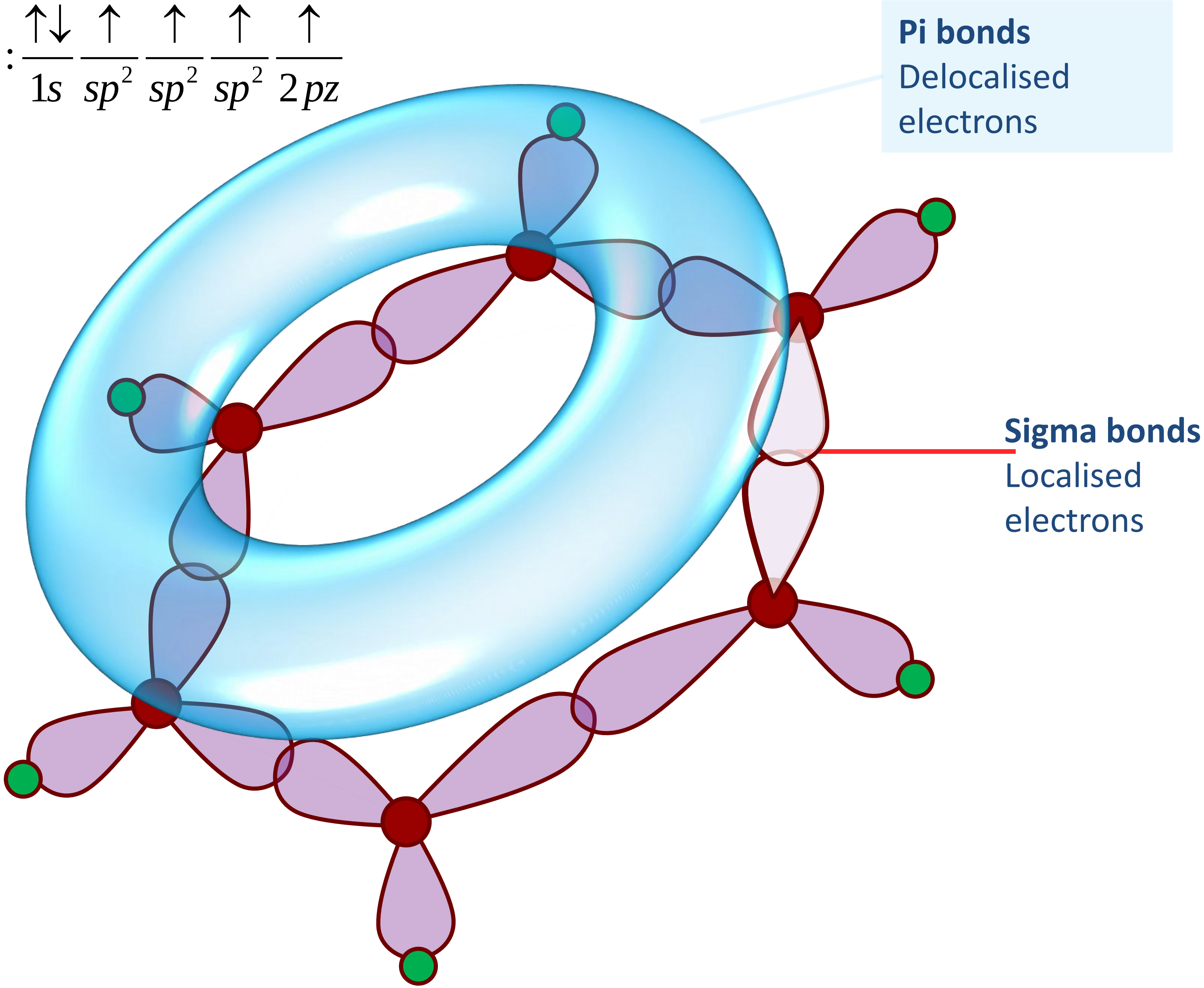
1. What is graphene?



Graphene is a 2D sheet of carbon atoms with record electrical and thermal conductivity, mechanical strength, stability, impermeability.

$$C_{sp2}:\frac{\uparrow\downarrow}{1s}\ \frac{\uparrow}{sp^2}\ \frac{\uparrow}{sp^2}\ \frac{\uparrow}{sp^2}\ \frac{\uparrow}{2pz}$$





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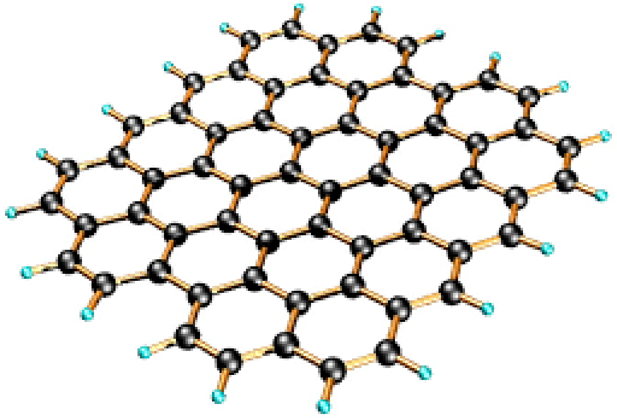
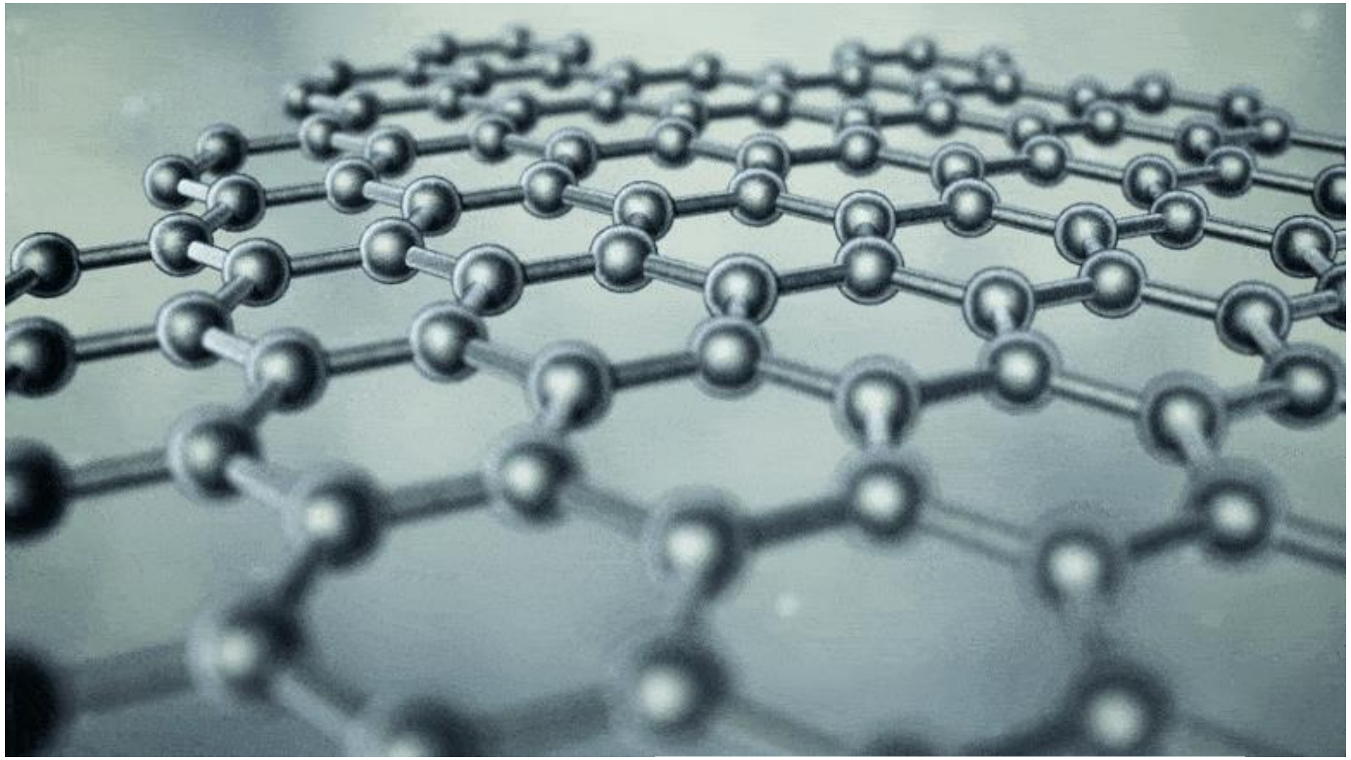
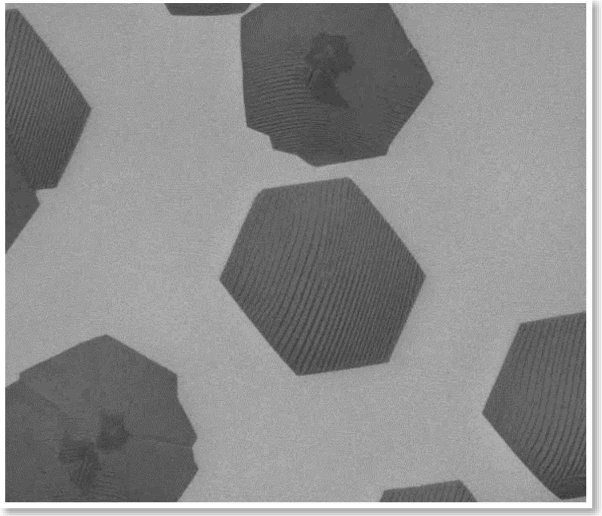
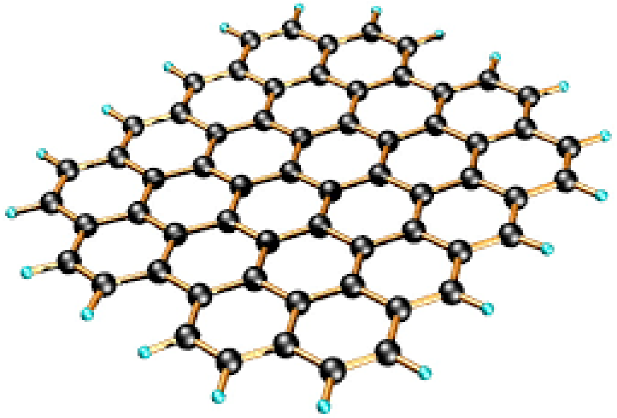
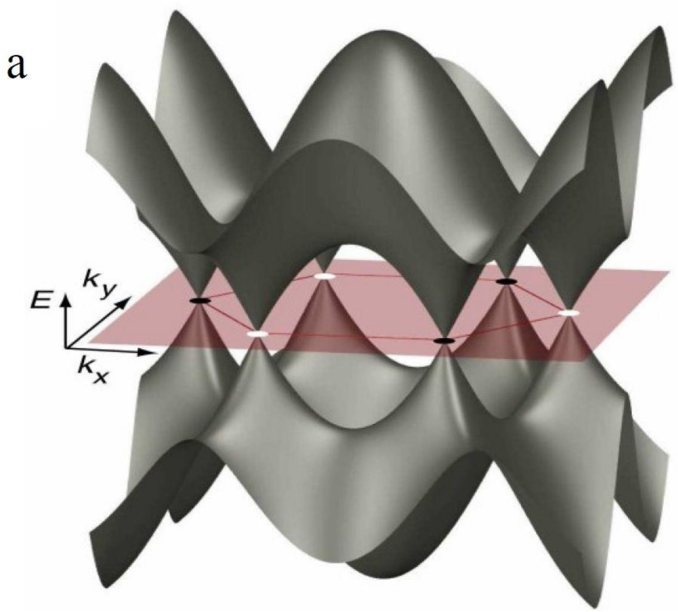




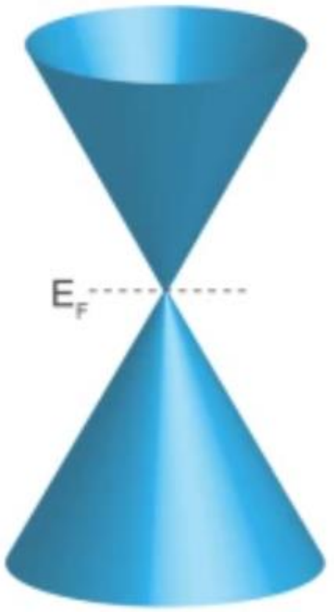
Graphene is a 2D sheet of carbon atoms with record electrical and thermal conductivity, mechanical strength, stability, impermeability.







Beenakker, Rev Mod Phys, 80 (2008), 1337



Graphene is a 2D sheet of carbon atoms with record electrical and thermal conductivity, mechanical strength, stability, impermeability.

Graphene is a zero-bandgap semiconductor with a linear dispersion :

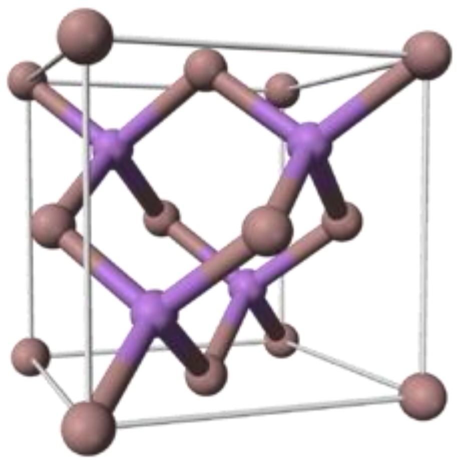
$$E_F = c^*p = v_F \cdot \hbar k_F$$

Graphene electrons are massless relativistic quasiparticles, travelling at the ”speed of light”

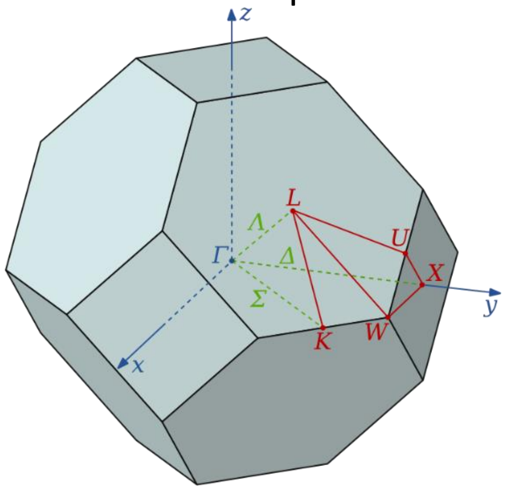
$$v_F = \frac{c}{300}$$

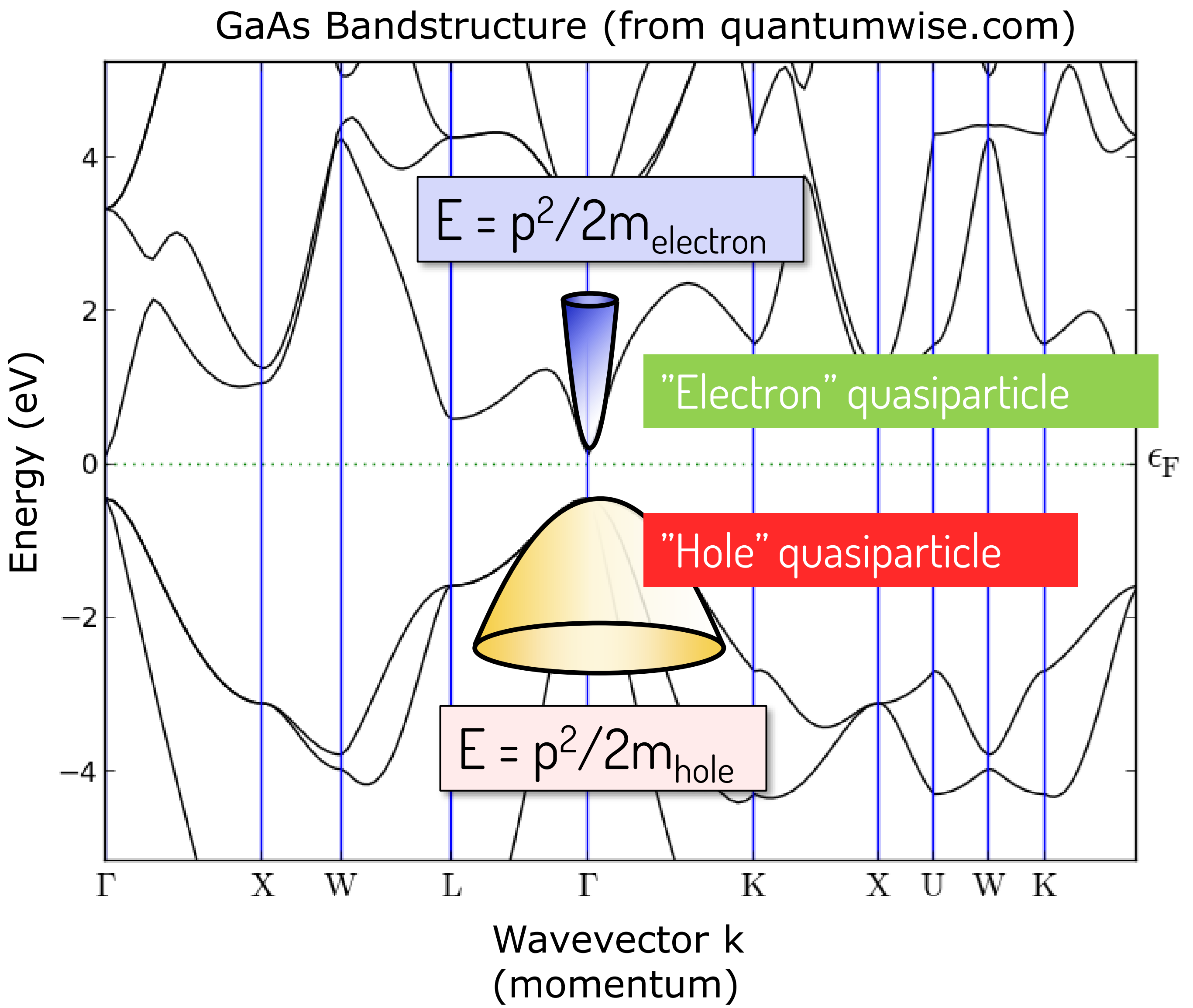
A ”free” electron in a semiconductor – a ”quasiparticle”

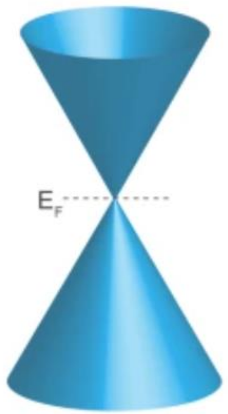
Real space

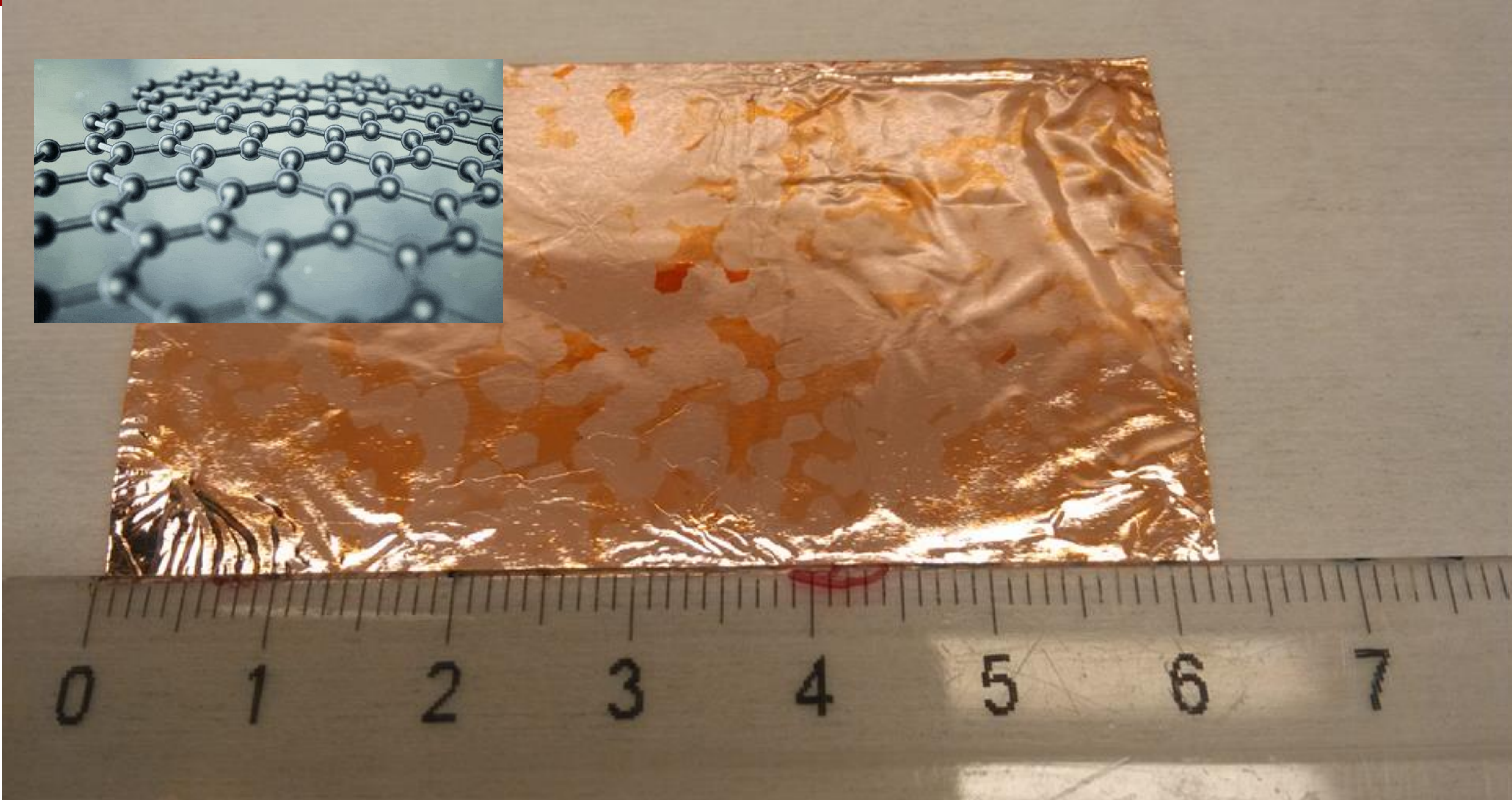


Momentum space

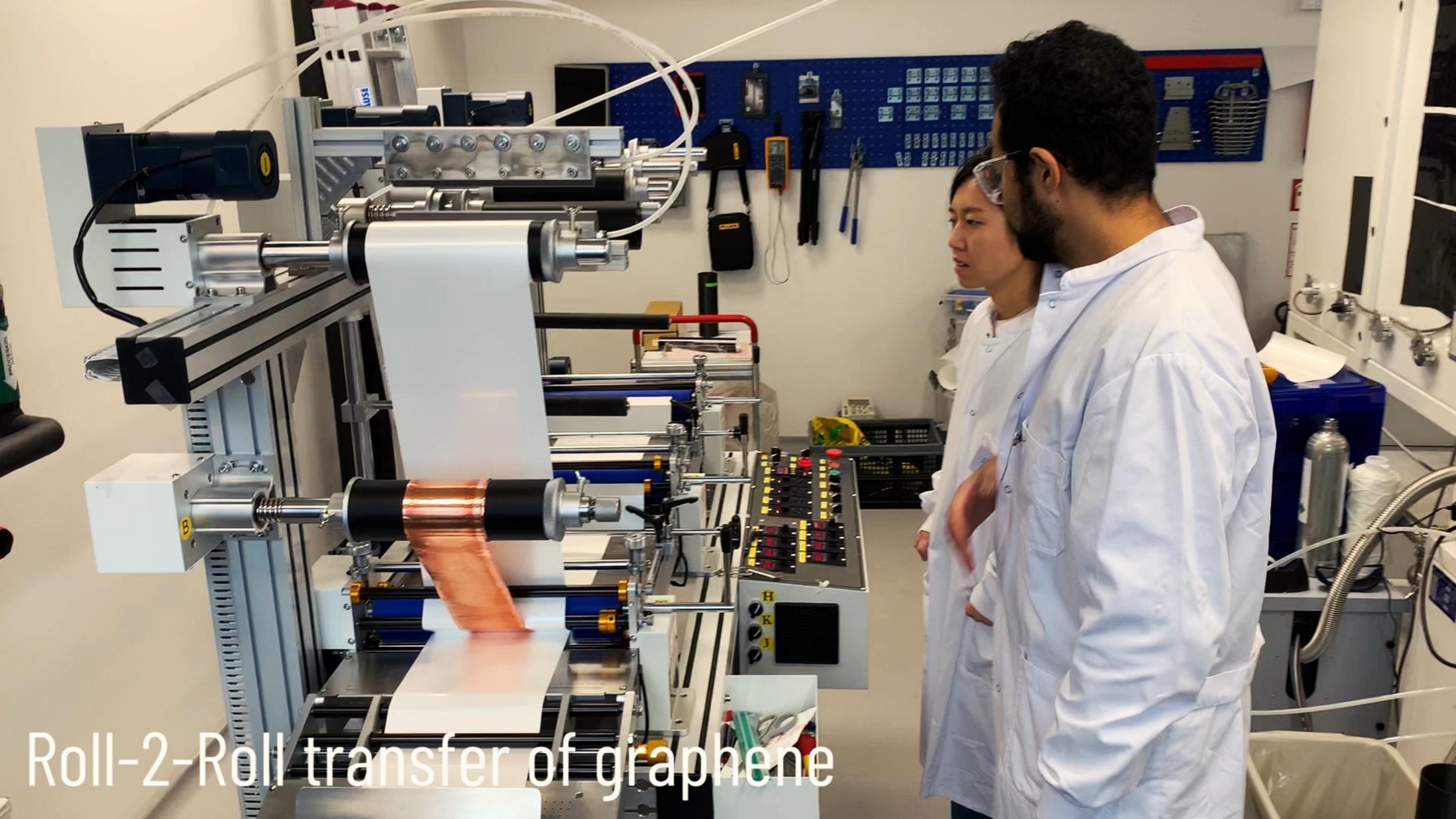




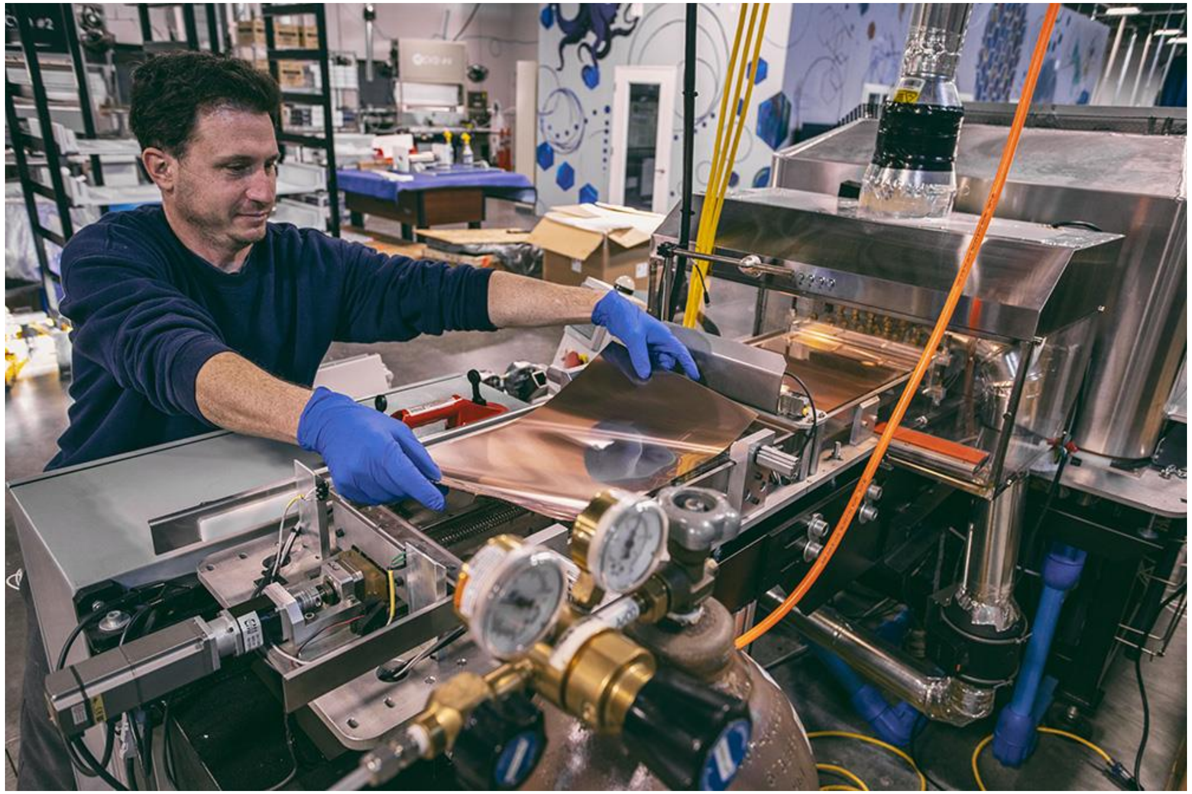


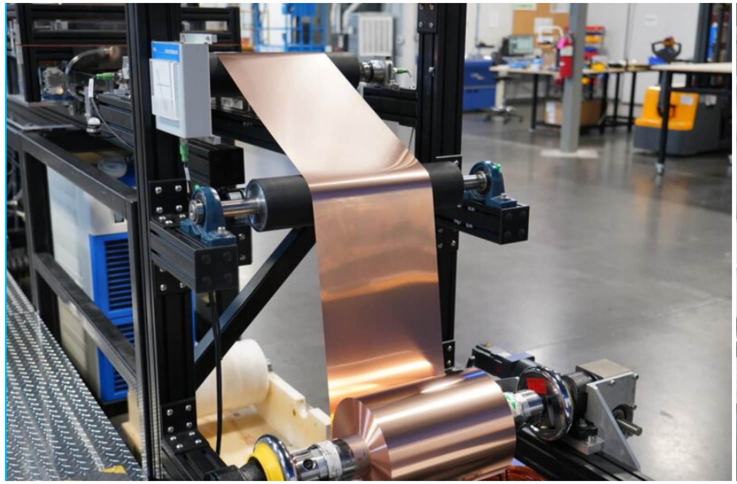


Birong Luo og Tim Booth, DTU Nanotech


Roll-2-Roll transfer of graphene

Graphene is being scaled as we speak

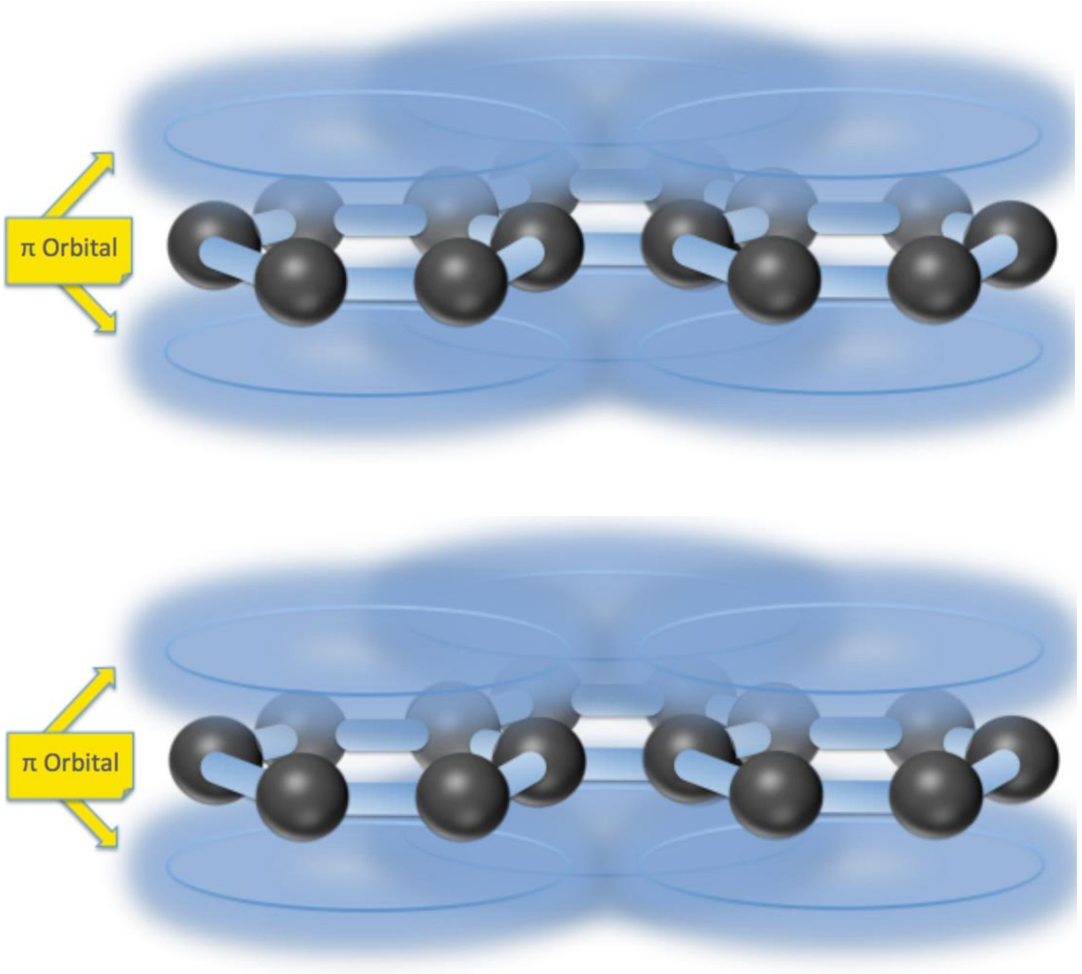


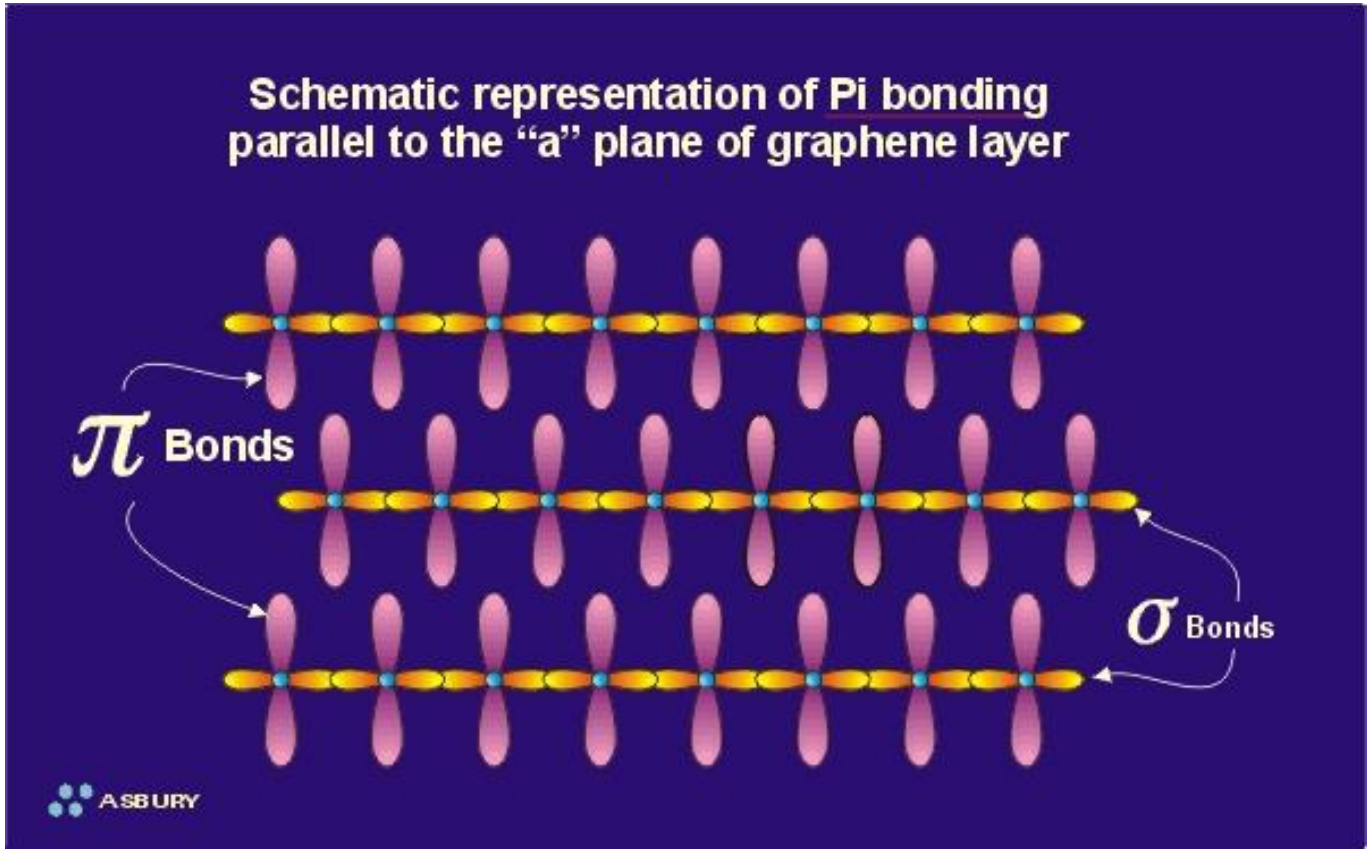


GENERAL GRAPHENE

2. 2D van der Waals epitaxy

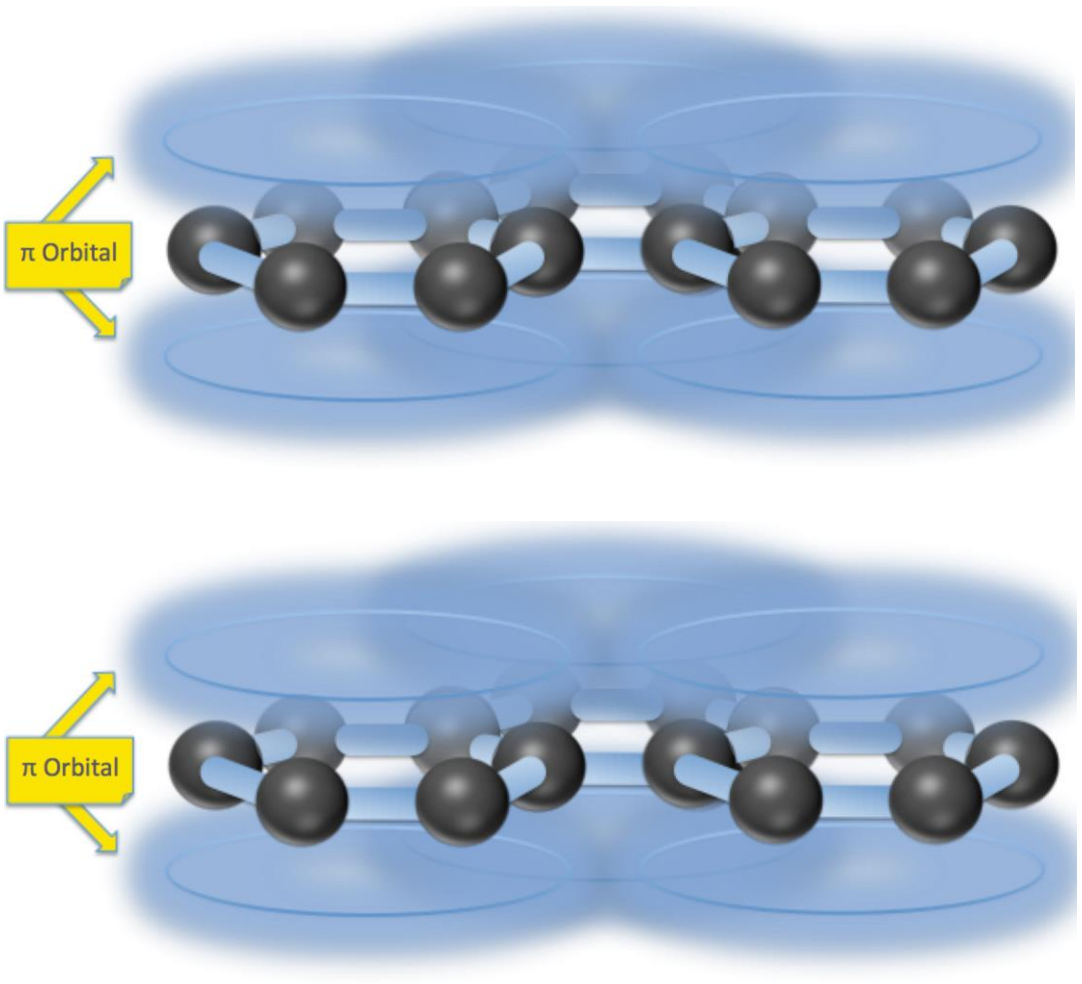
Graphene: π-resonant electrons → π–electrons can hop between atoms

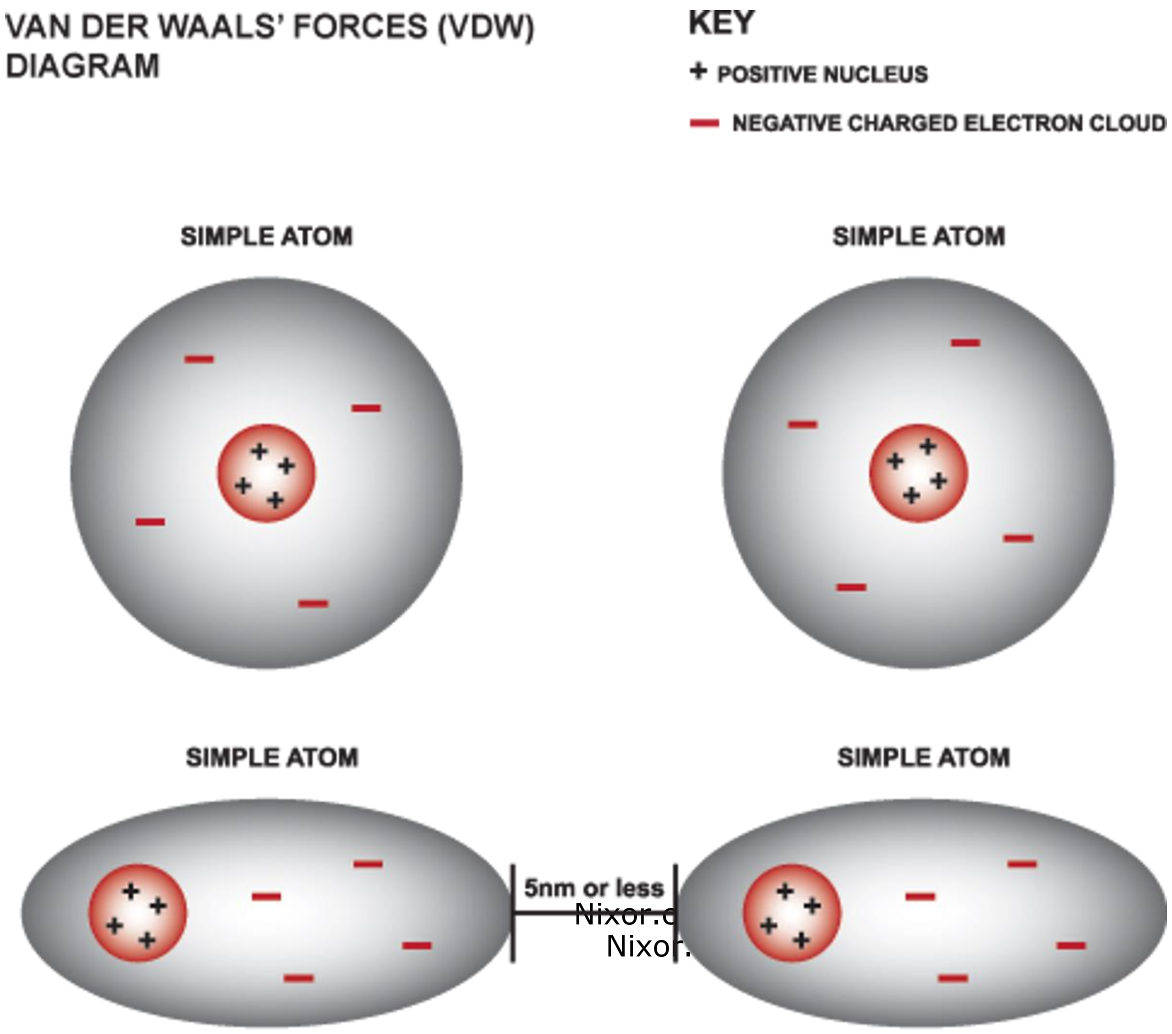




What special properties does graphene have?

Graphene: π-resonant electrons → π–electrons can hop between atoms





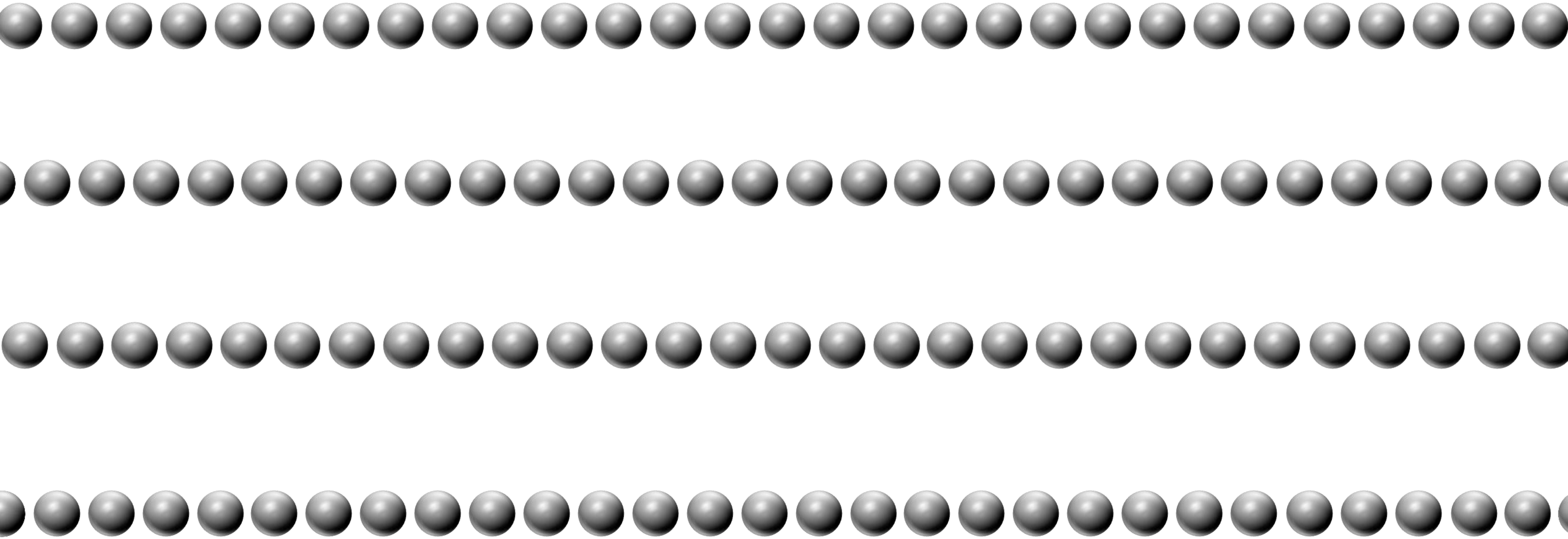
When two atoms come within 5 nanometers of each other, there will be a slight interaction between them, thus causing polarity and a slight attraction.

Van der Waals forces – heterostructures

$$W_{ab} = -\frac{C_{orient} + C_{ind} + C_{disp}}{r^6} = -\frac{C}{r^6}$$

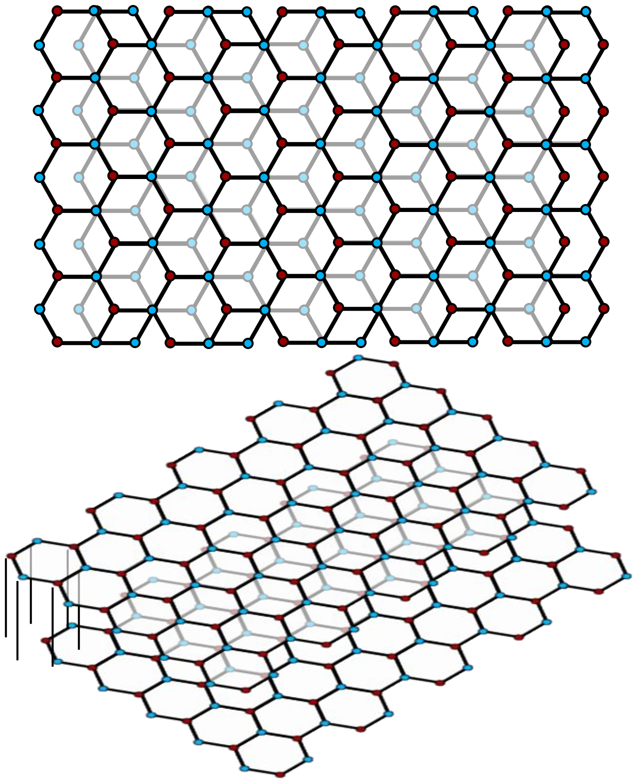
$$W_{AB} = \sum_{i,j} \frac{C_{vdW}}{r^6_{ij}}$$

$$W_{AB} = -\frac{C_{ab}}{r_{ab}^6} \cdot dV_A \rho_A \cdot dV_B \rho_B$$

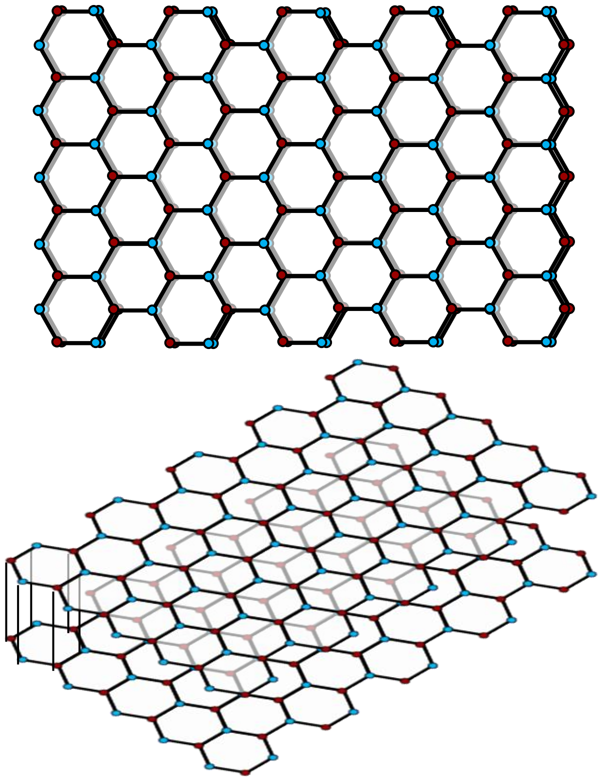


AB, AA and turbostratic stacking

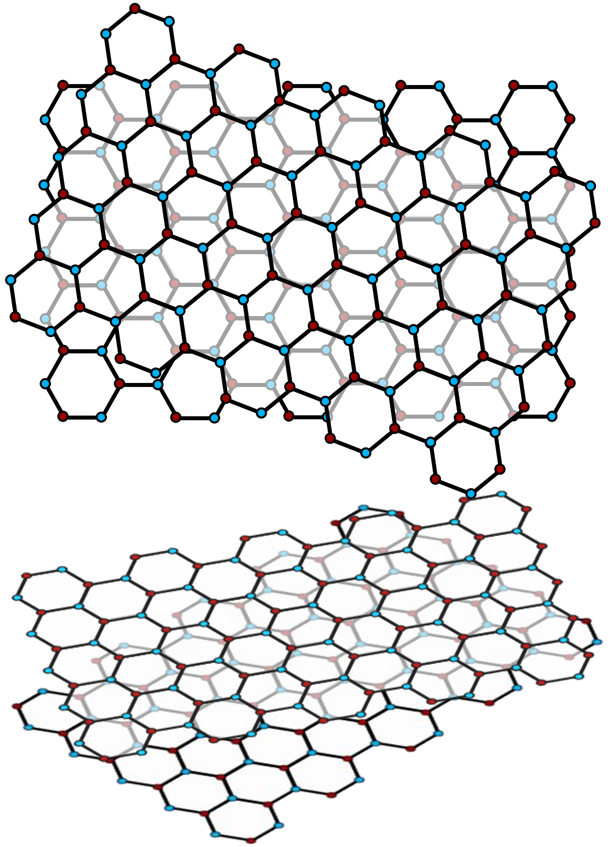
AB stacked

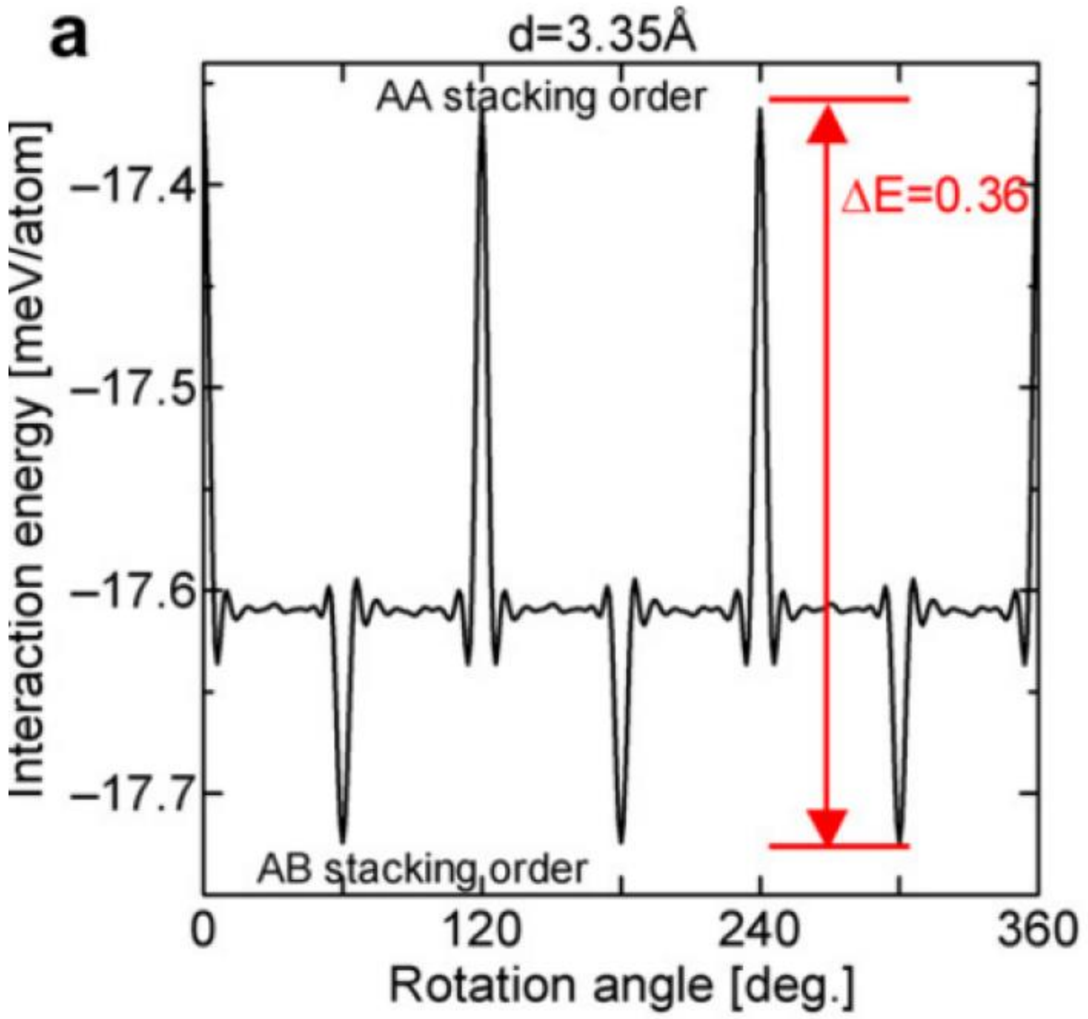


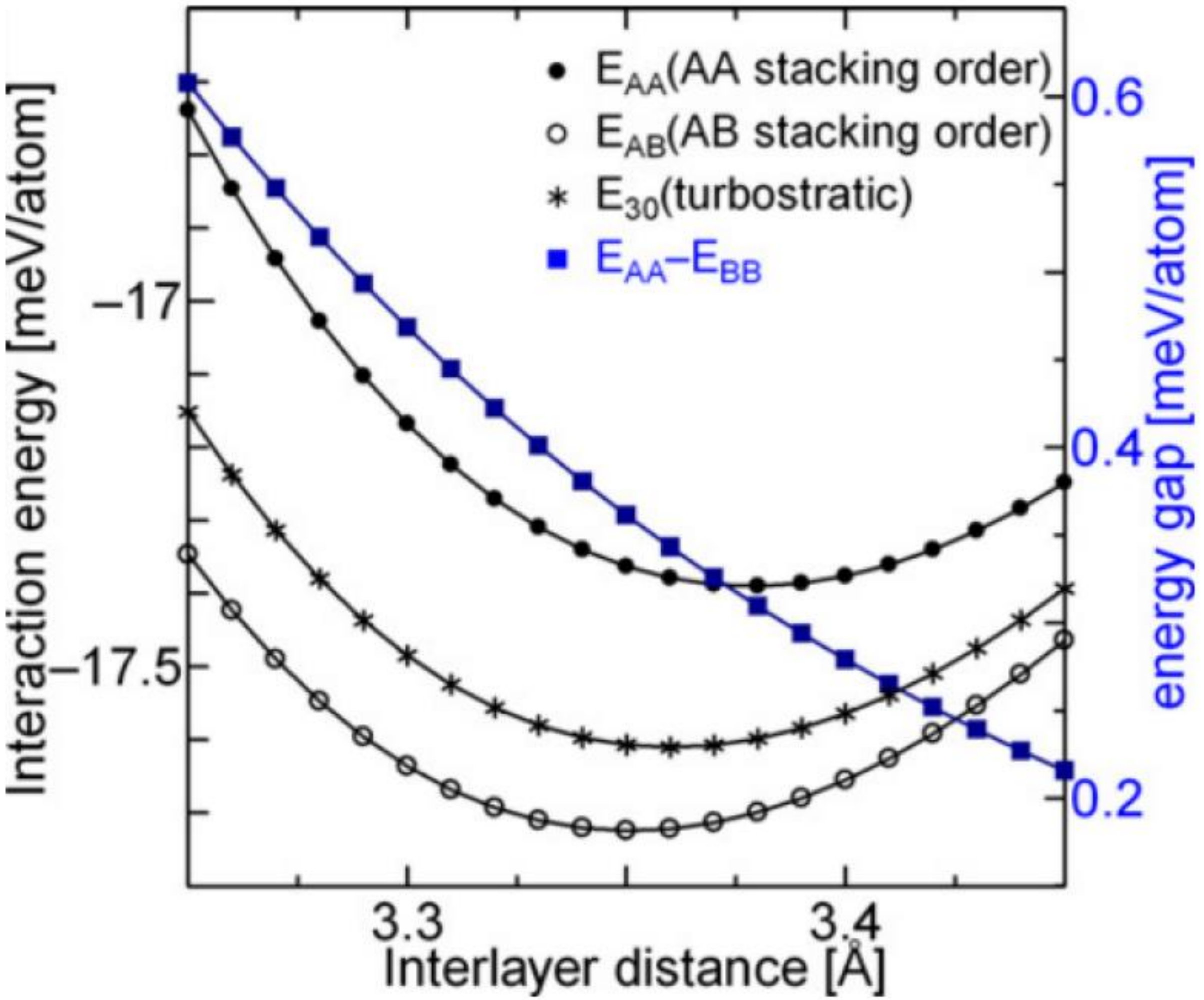
AA stacked



Turbostratic/Twisted







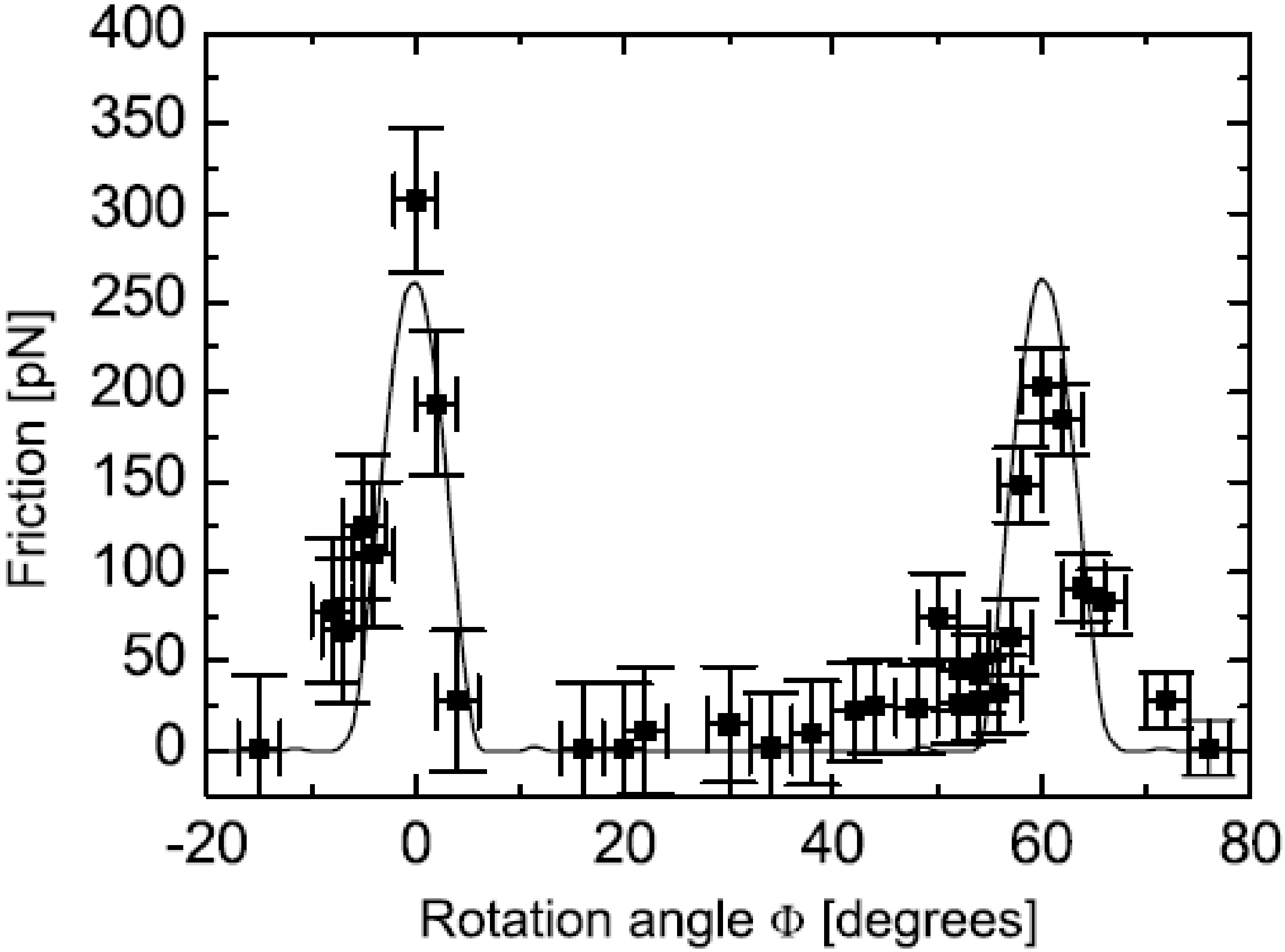
Chemical Physics Letters **2011,** *512* (4-6), 146-150.

Superlubricity

VOLUME 92, NUMBER 12 PHYSICAL REVIEW LETTERS week ending 26 MARCH 2004

Superlubricity of Graphite

Martin Dienwiebel,* Gertjan S. Verhoeven, Namboodiri Pradeep, and Joost W. M. Frenken†
Kamerlingh Onnes Laboratory, Leiden University, P.O. Box 9504, 2300 RA Leiden, The Netherlands



NANO LETTERS

Letter

pubs.acs.org/NanoLett

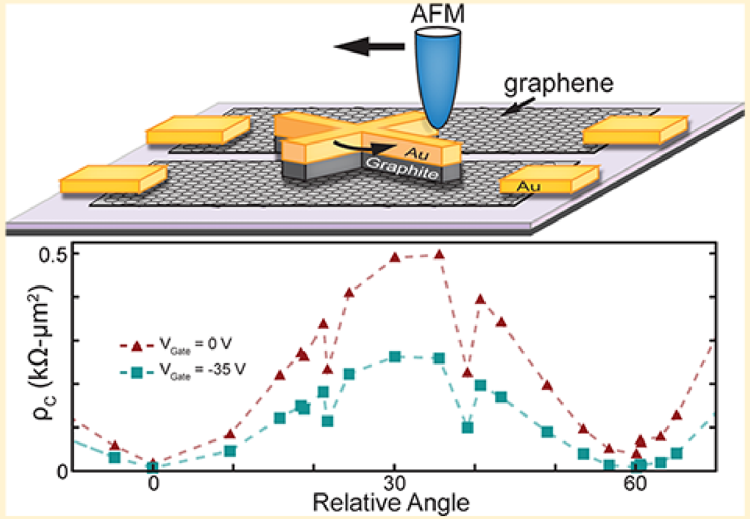
Resistivity of Rotated Graphite–Graphene Contacts

Tarun Chari,[†] Rebeca Ribeiro-Palau,[‡] Cory R. Dean,[‡] and Kenneth Shepard*[,†]

[†]Department of Electrical Engineering and [‡]Department of Physics, Columbia University, New York, New York 10027, United States

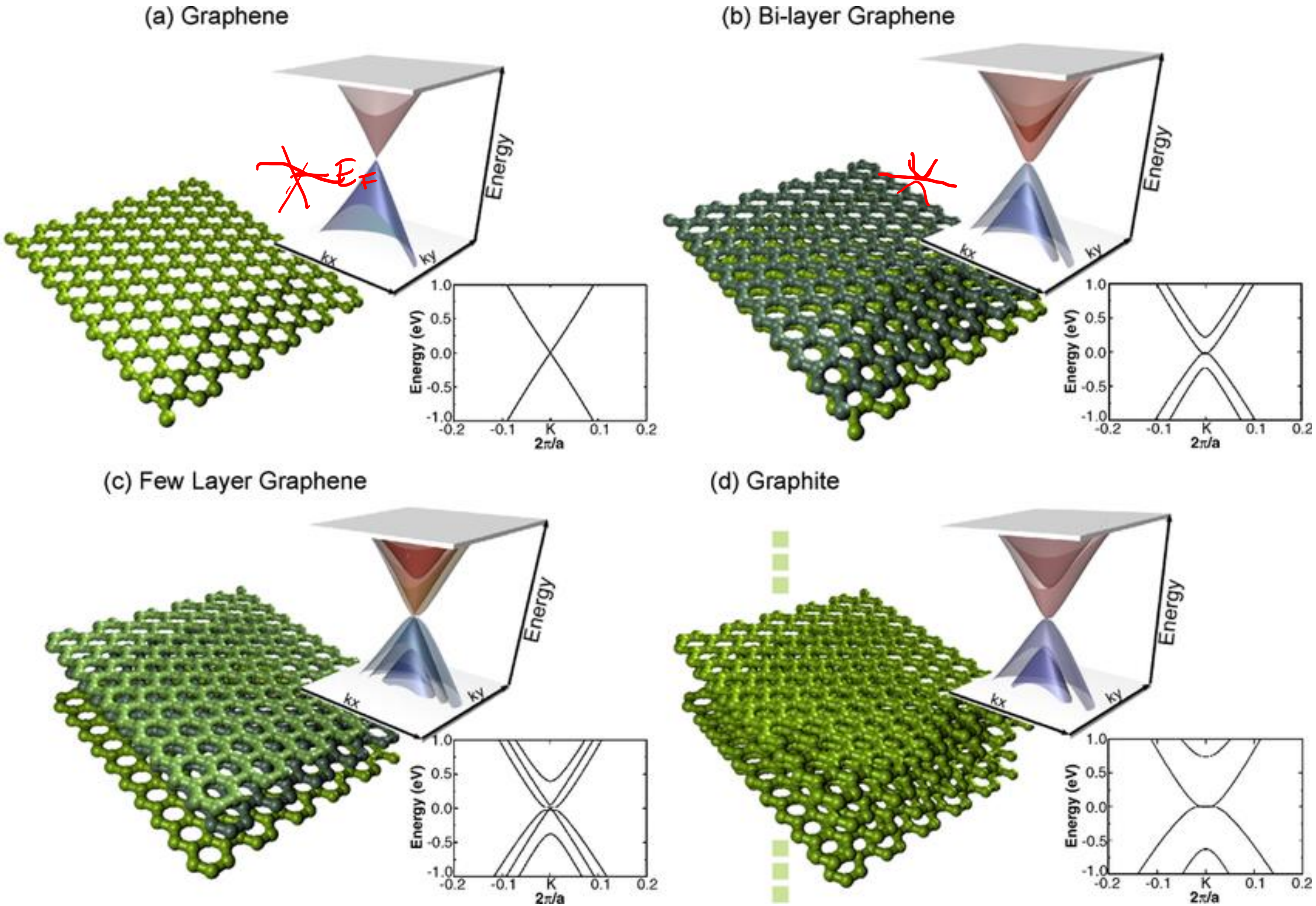
Ⓢ *Supporting Information*

ABSTRACT: Robust electrical contact of bulk conductors to two-dimensional (2D) material, such as graphene, is critical to the use of these 2D materials in practical electronic devices. Typical metallic contacts to graphene, whether edge or areal, yield a resistivity of no better than 100 Ω μm but are typically >10 kΩ μm. In this Letter, we employ single-crystal graphite for the bulk contact to graphene instead of conventional metals. The graphite contacts exhibit a transfer length up to four-times longer than in conventional metallic contacts. Furthermore, we are able to drive the contact resistivity to as little as 6.6 Ω μm^2 by tuning the relative orientation of the graphite and graphene crystals. We find that the contact resistivity exhibits a 60° periodicity corresponding to crystal symmetry with additional sharp decreases around 22° and 39°, which are among the commensurate angles of twisted bilayer graphene.

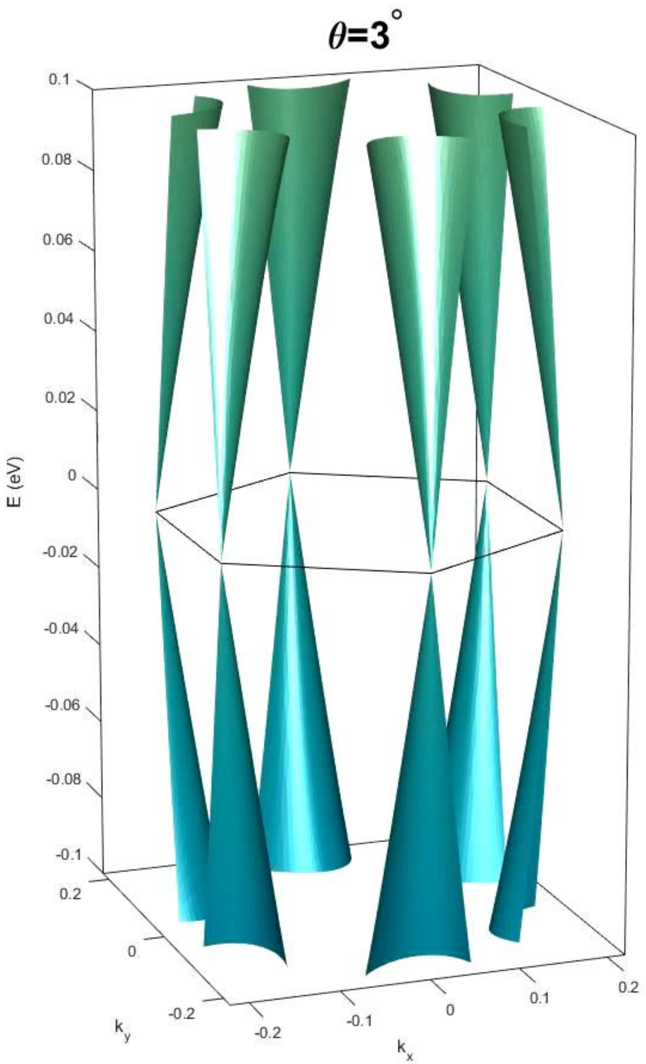


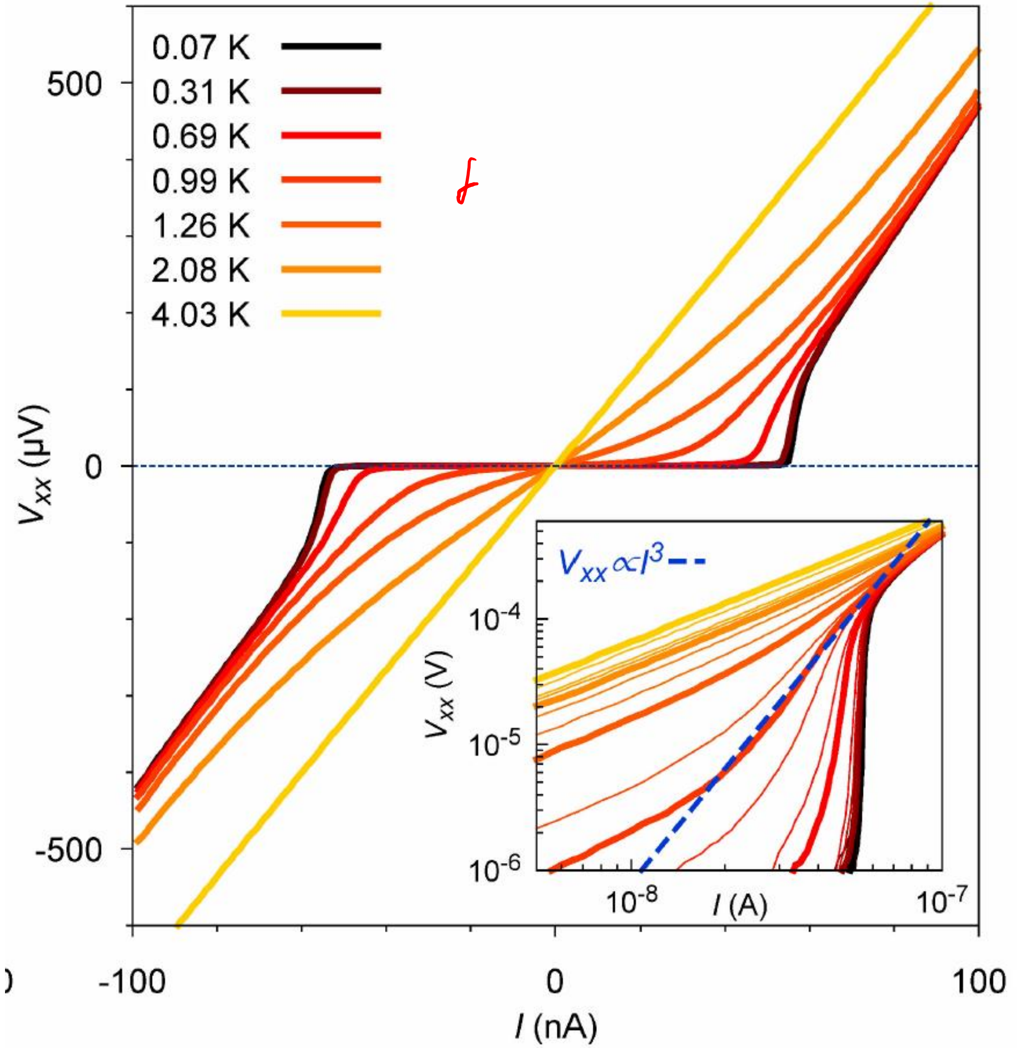
KEYWORDS: *Graphene, graphite, contact resistivity, commensurate angles*

AB, AA and turbostratic stacking



M. Terrones et al., Nano Today **5**, 351 (2010)

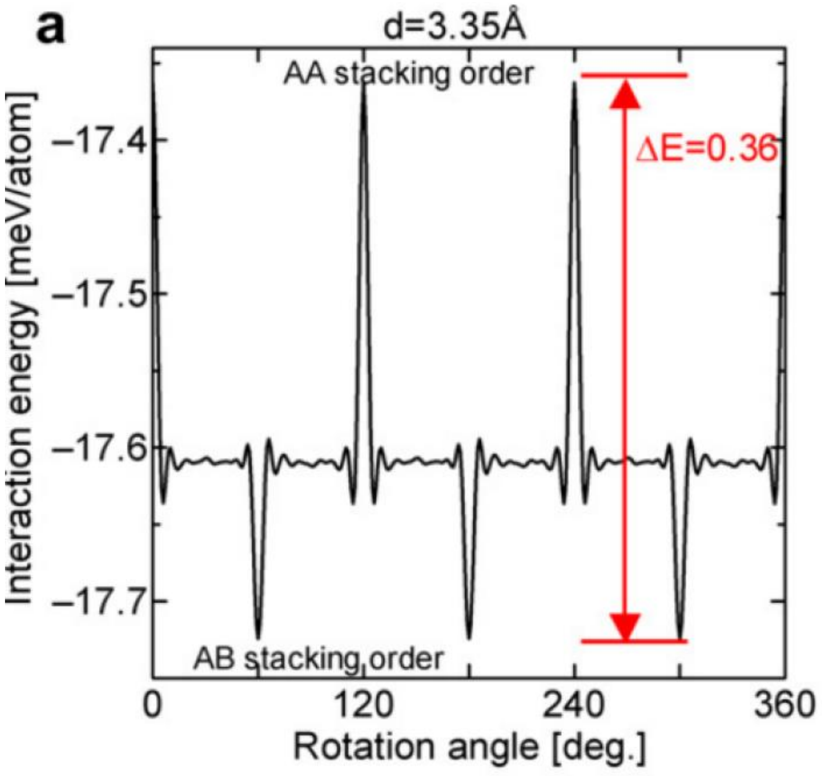


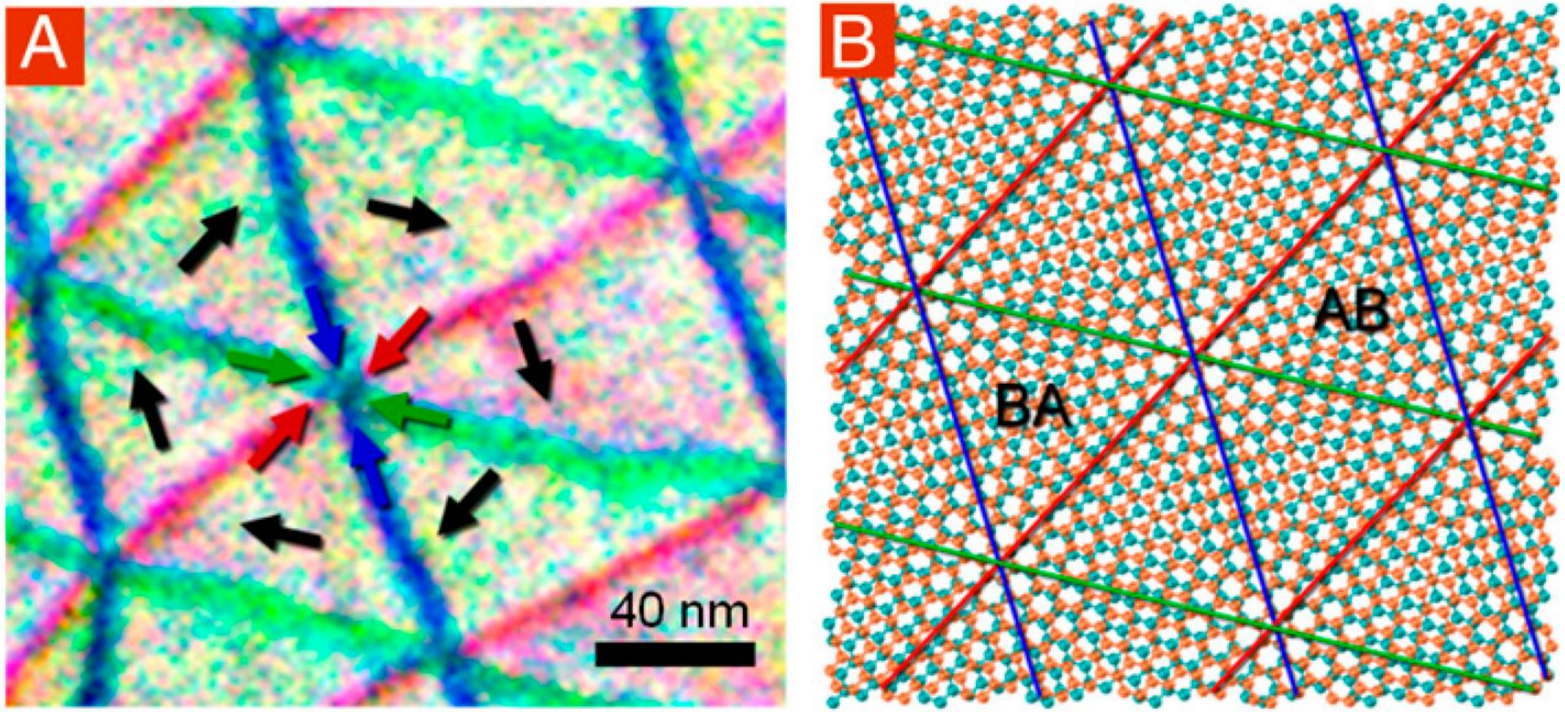


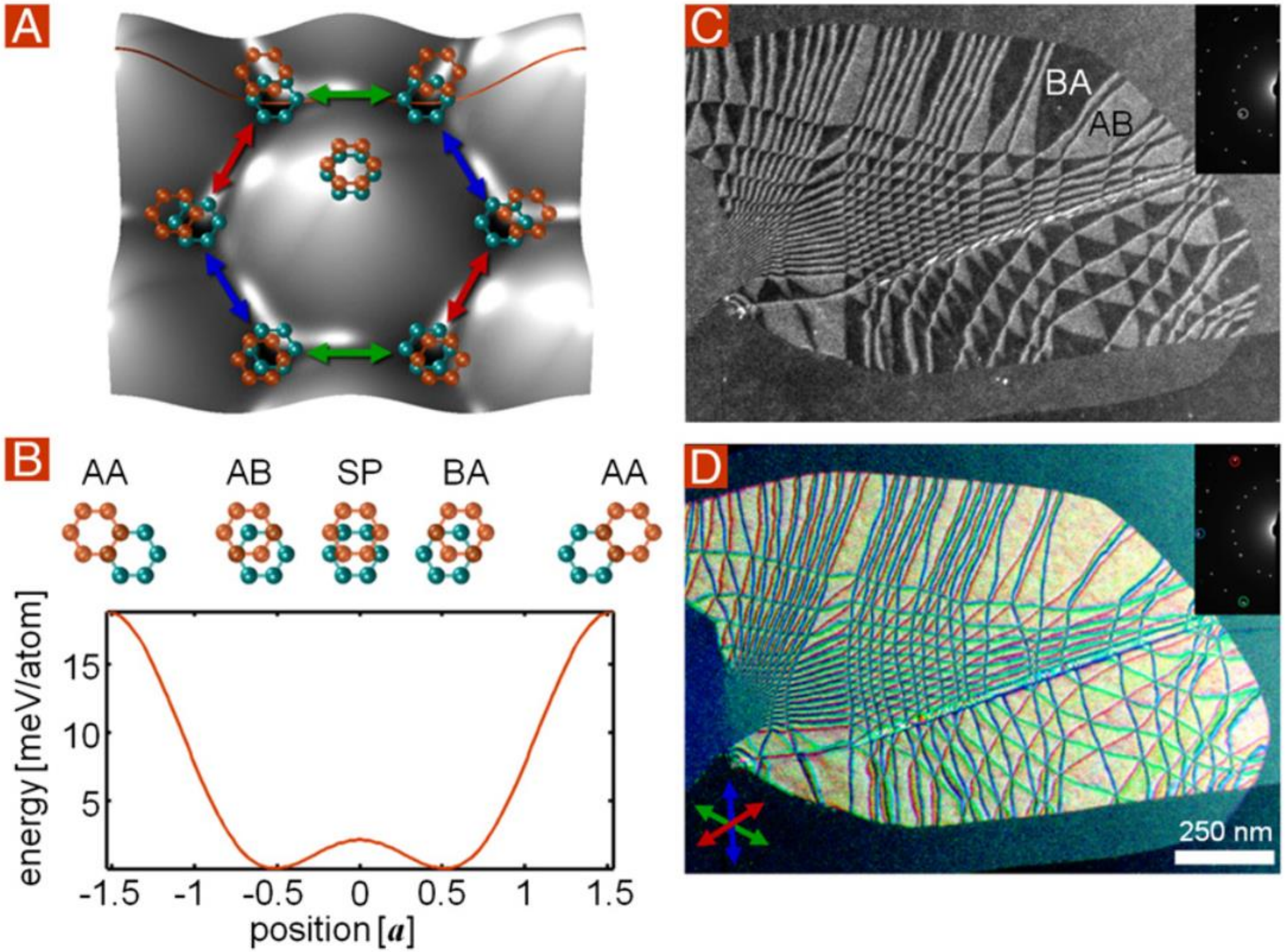
Cao, Nature **556**, pages 43–50, 2018

Strain solitons and topological defects in bilayer graphene

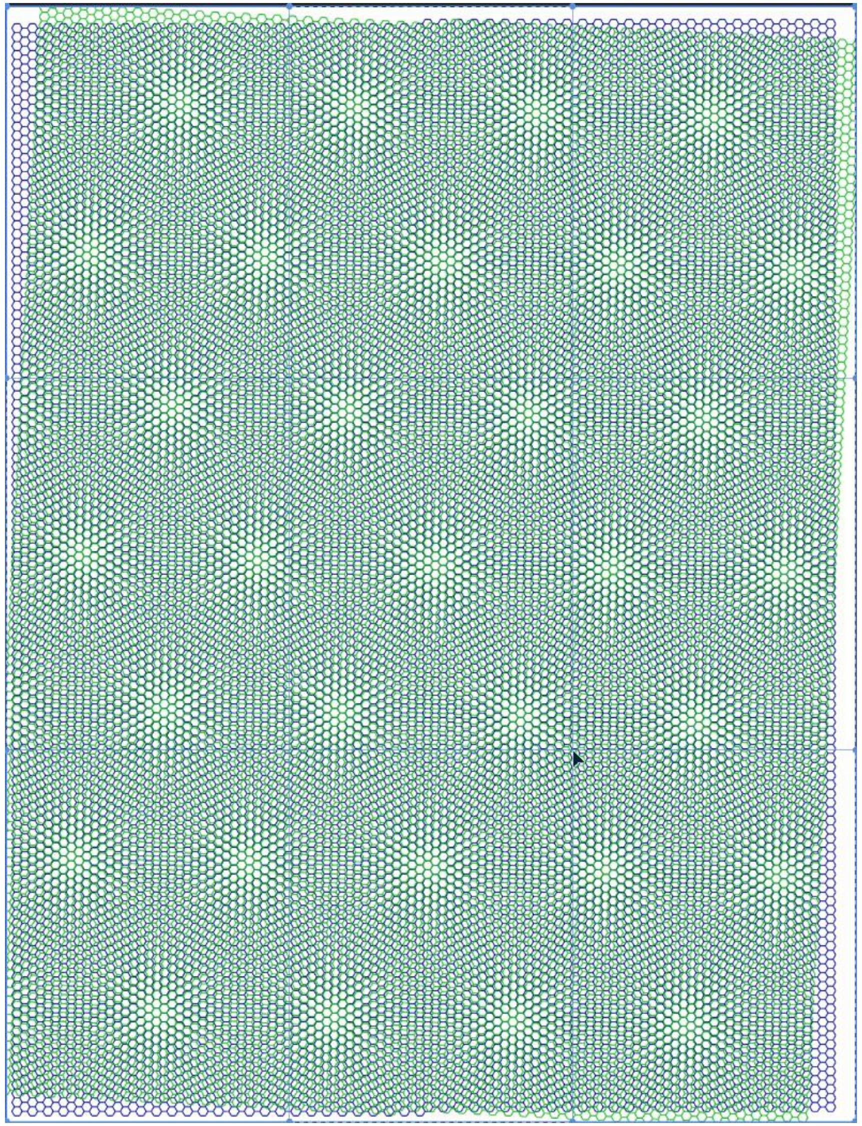
Jonathan S. Alden[a], Adam W. Tsen[a], Pinshane Y. Huang[a], Robert Hovden[a], Lola Brown[b], Jiwoong Park[b,c], David A. Muller[a,c], and Paul L. McEuen[c,d,1]



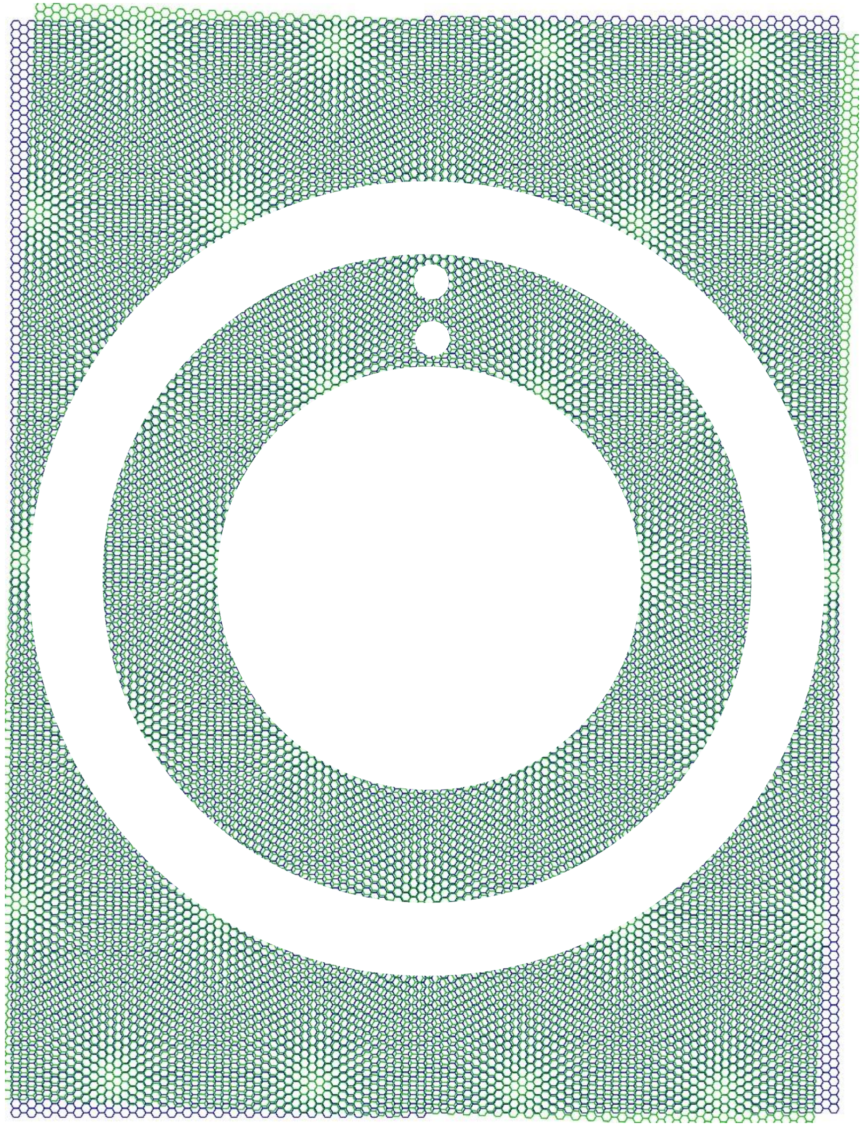



A
B
AA
AB
SP
BA
AA
energy [meV/atom]
15
10
5
-1.5
-1
-0.5
0
0.5
1
1.5
position [a]
C
BA
AB
D
250 nm

Challenges in using vdW epitaxy for engineering….

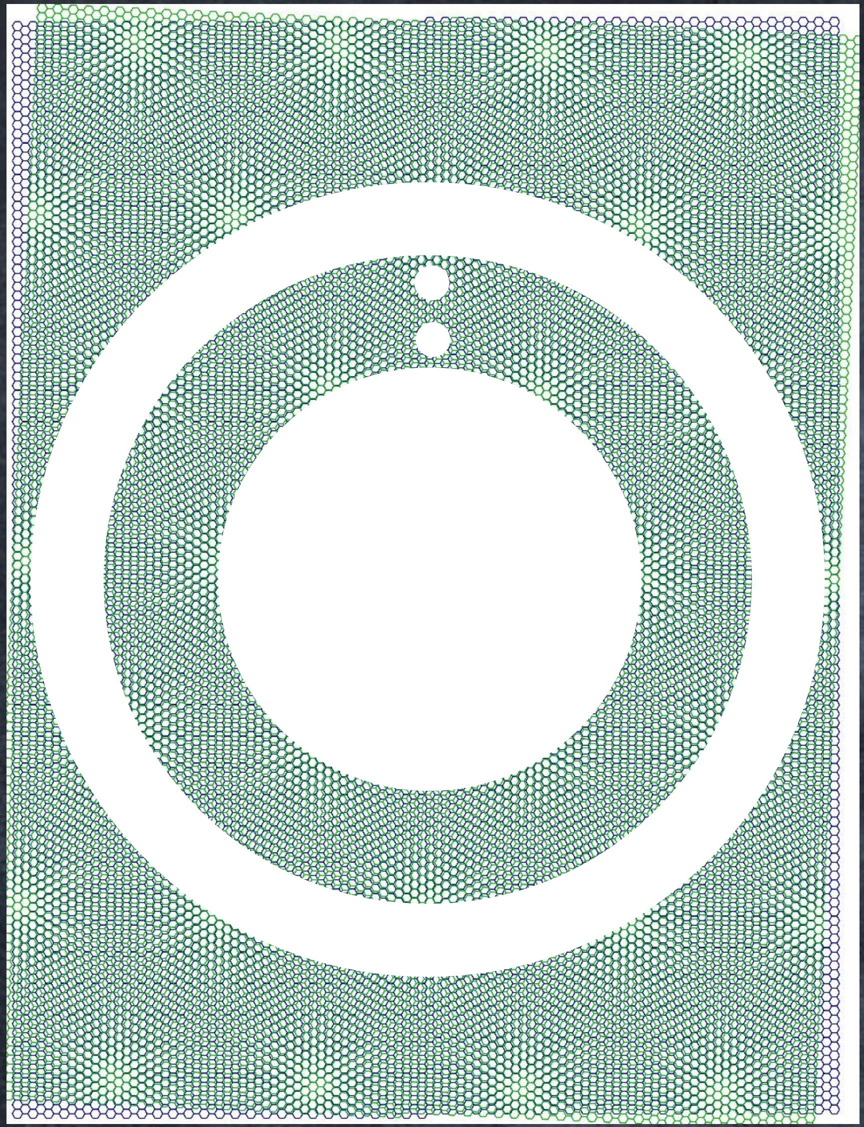


Upscaling



Patterning

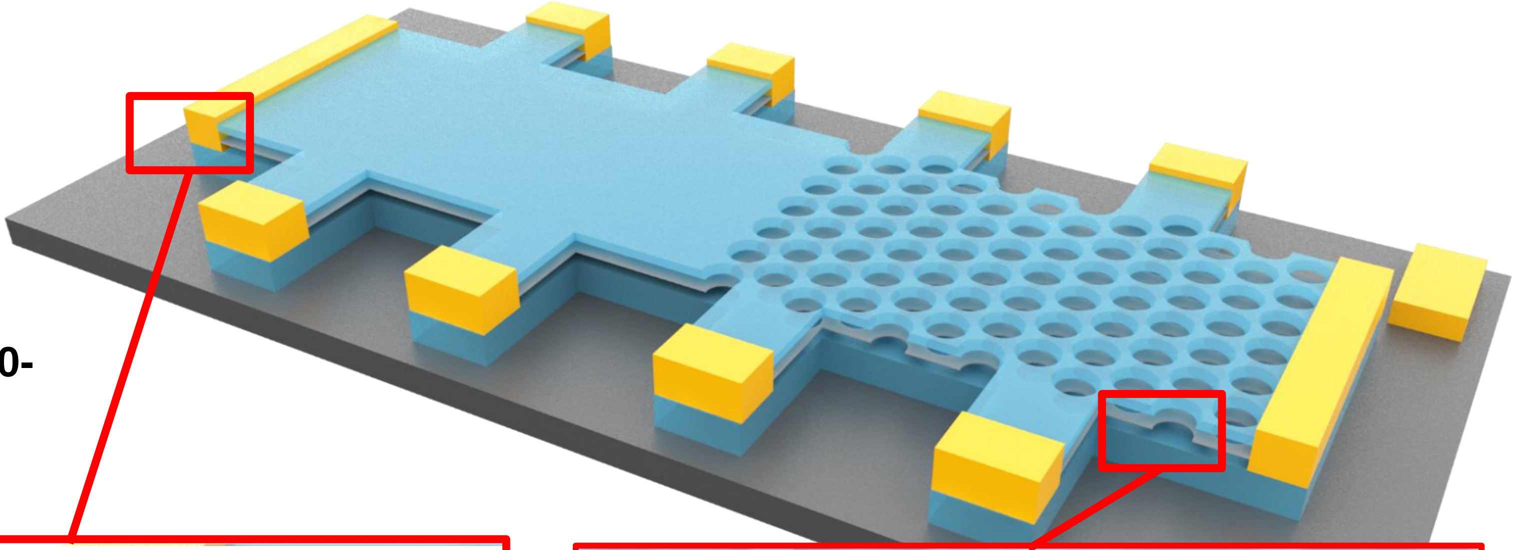
3. vdW epitaxy – patterning?

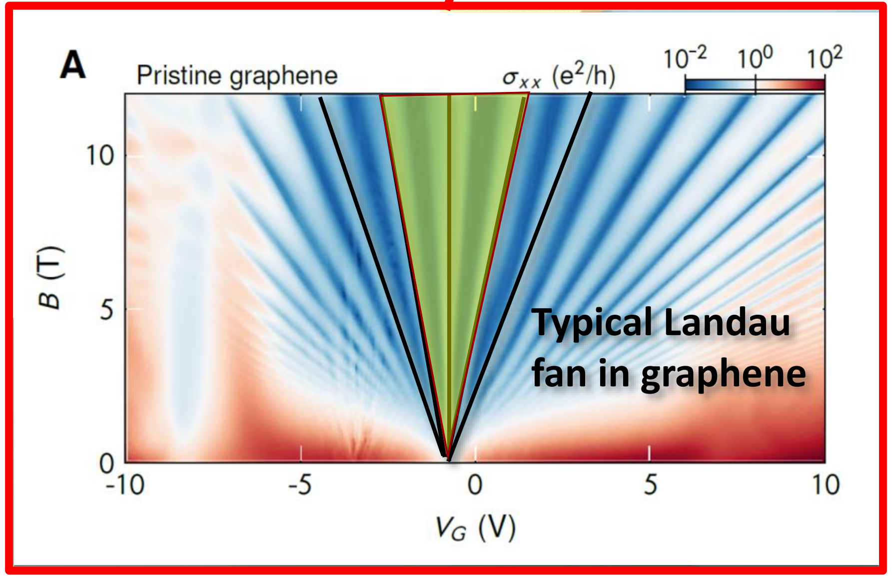


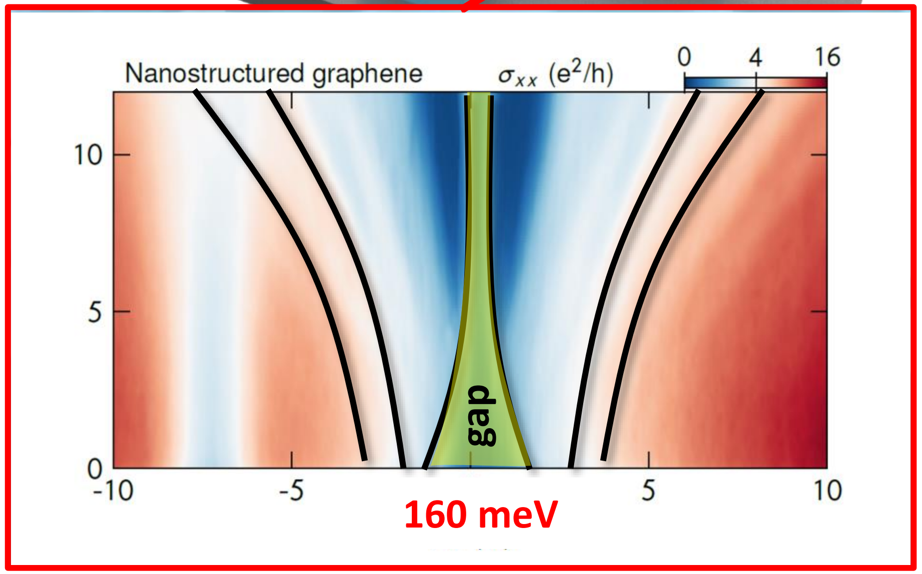
Nanopatterning through hBN

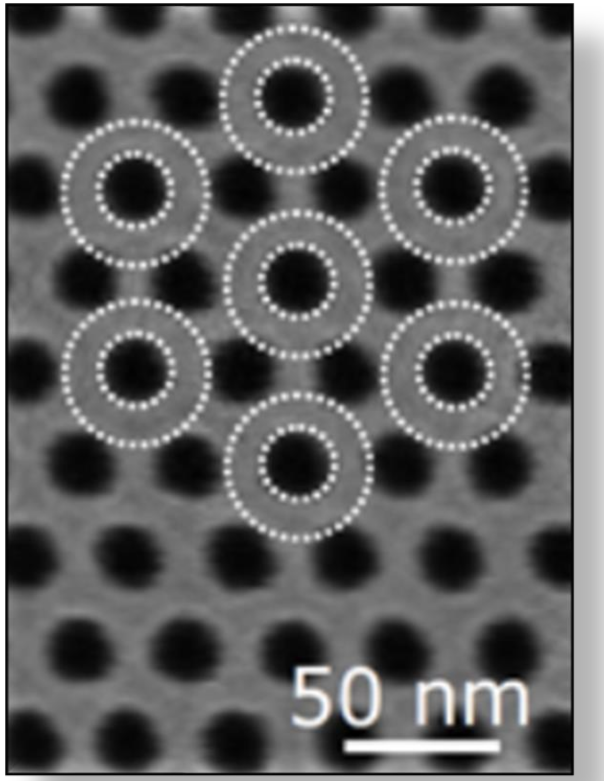
Mobility : 800 cm²/Vs

2 orders of magnitude better than for typical 10-15 nm constrictions



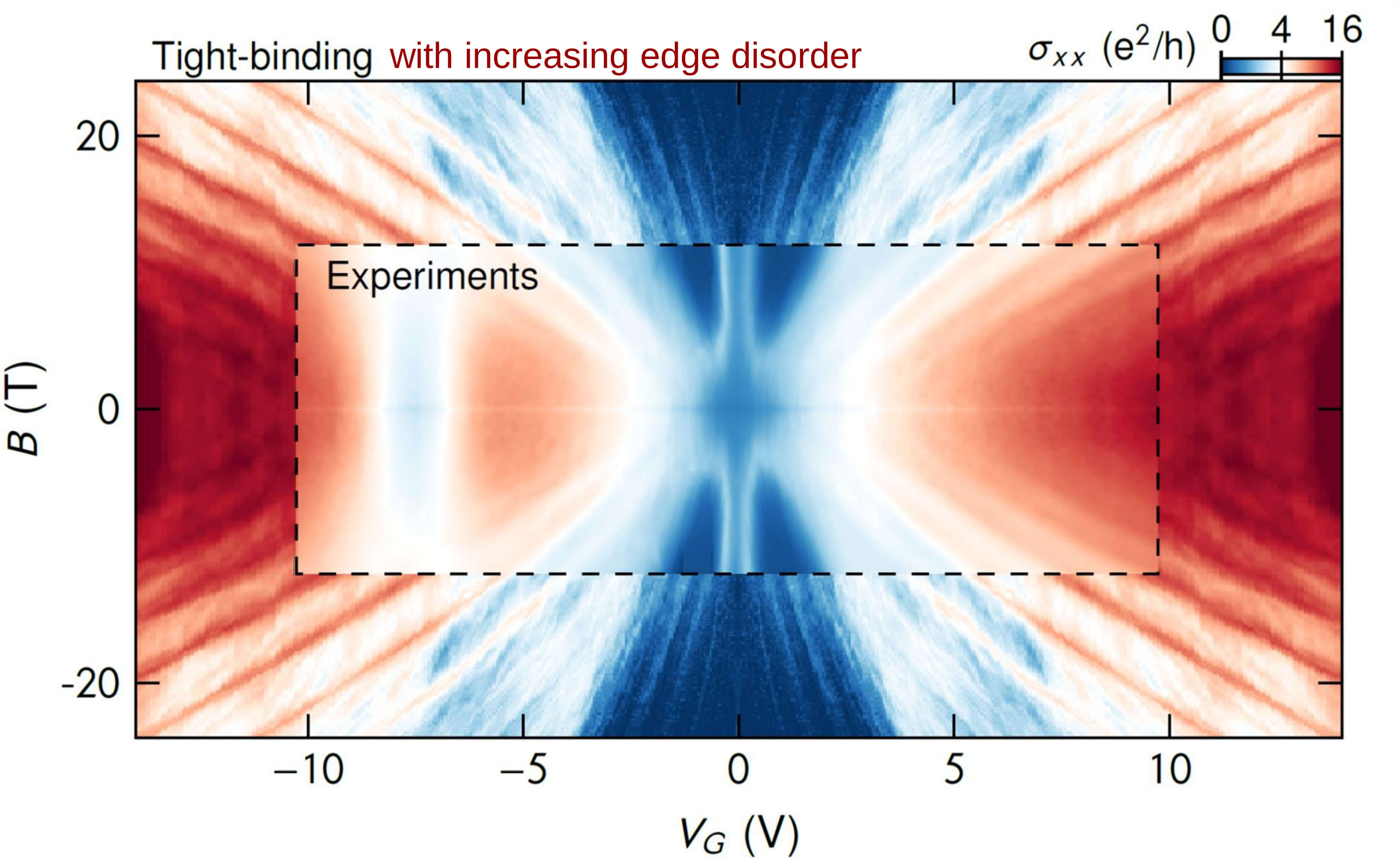






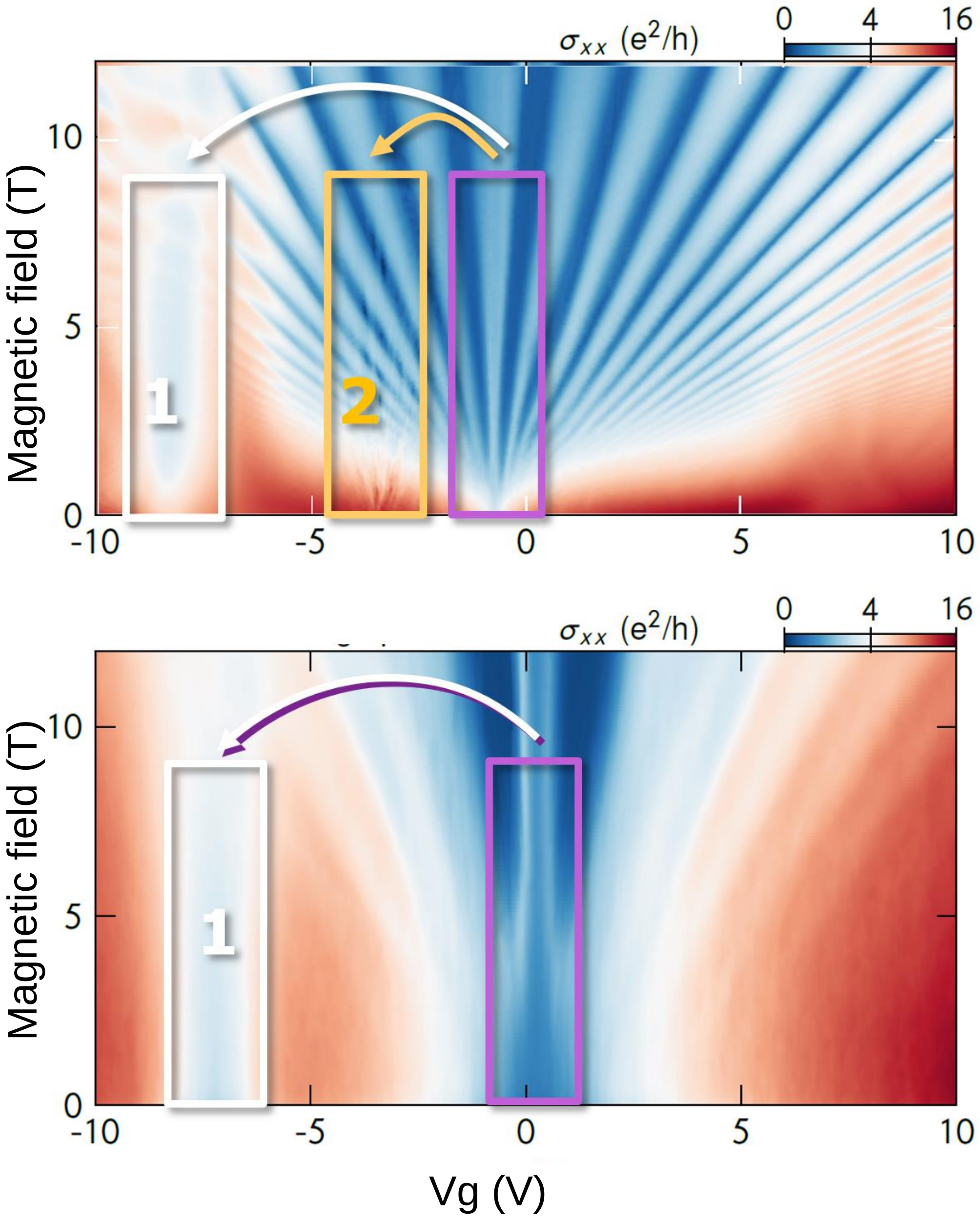
Jessen, Gammelgaard, Nature Nanotech. 14 340 (2019)

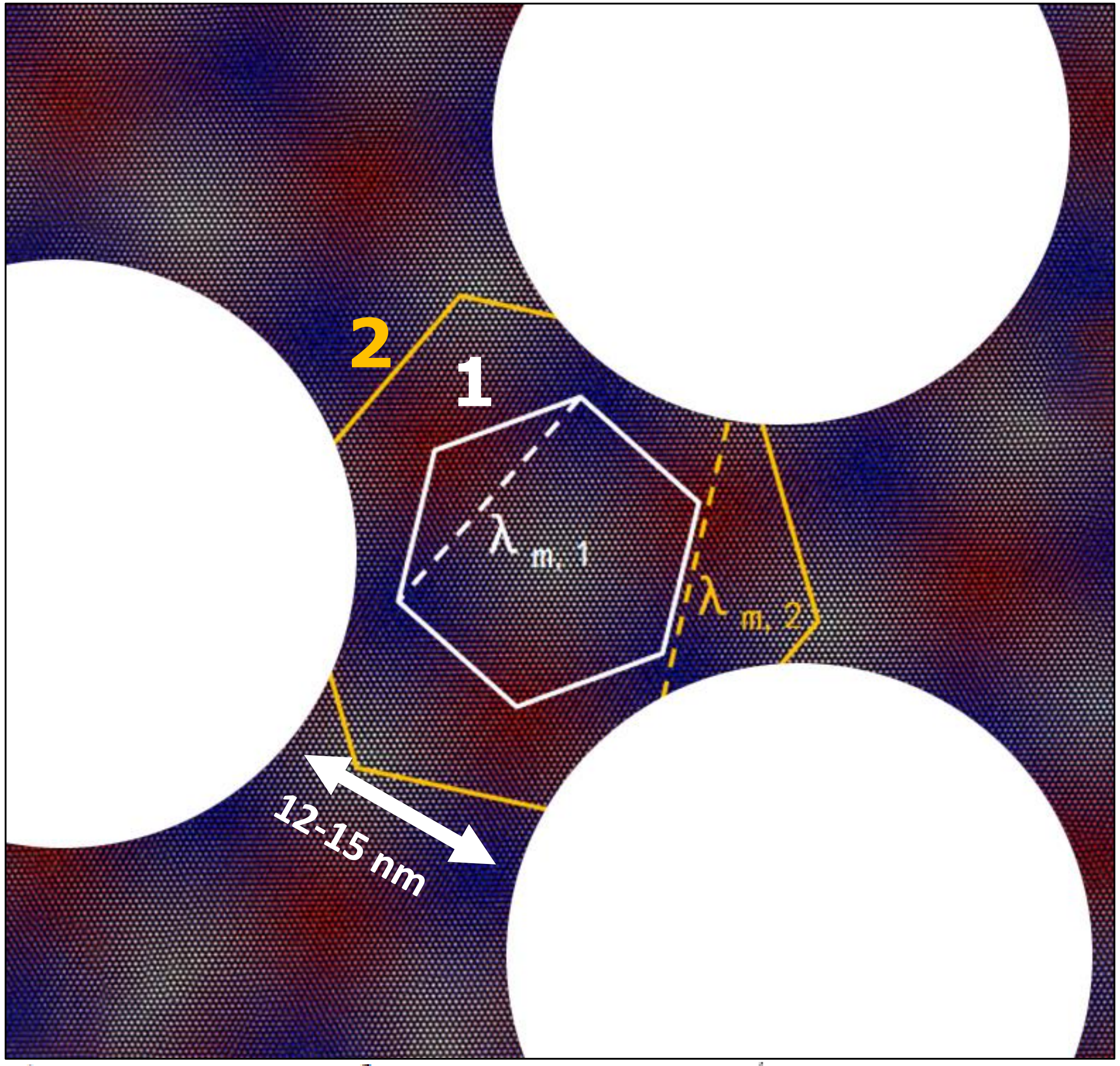
Experiment vs numerical and analytical predictions



Jessen, Gammelgaard, Nature Nanotech. 14 340 (2019)

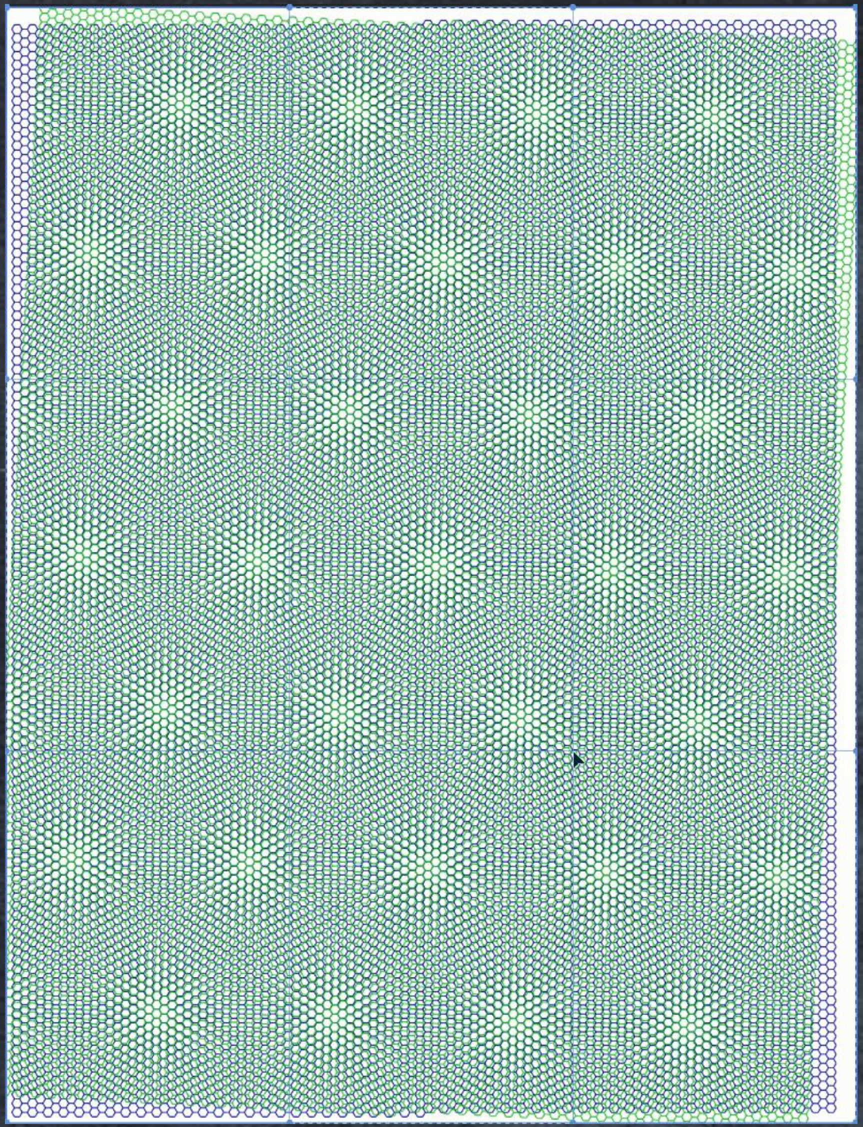
Moiré bandstructure – before and after patterning



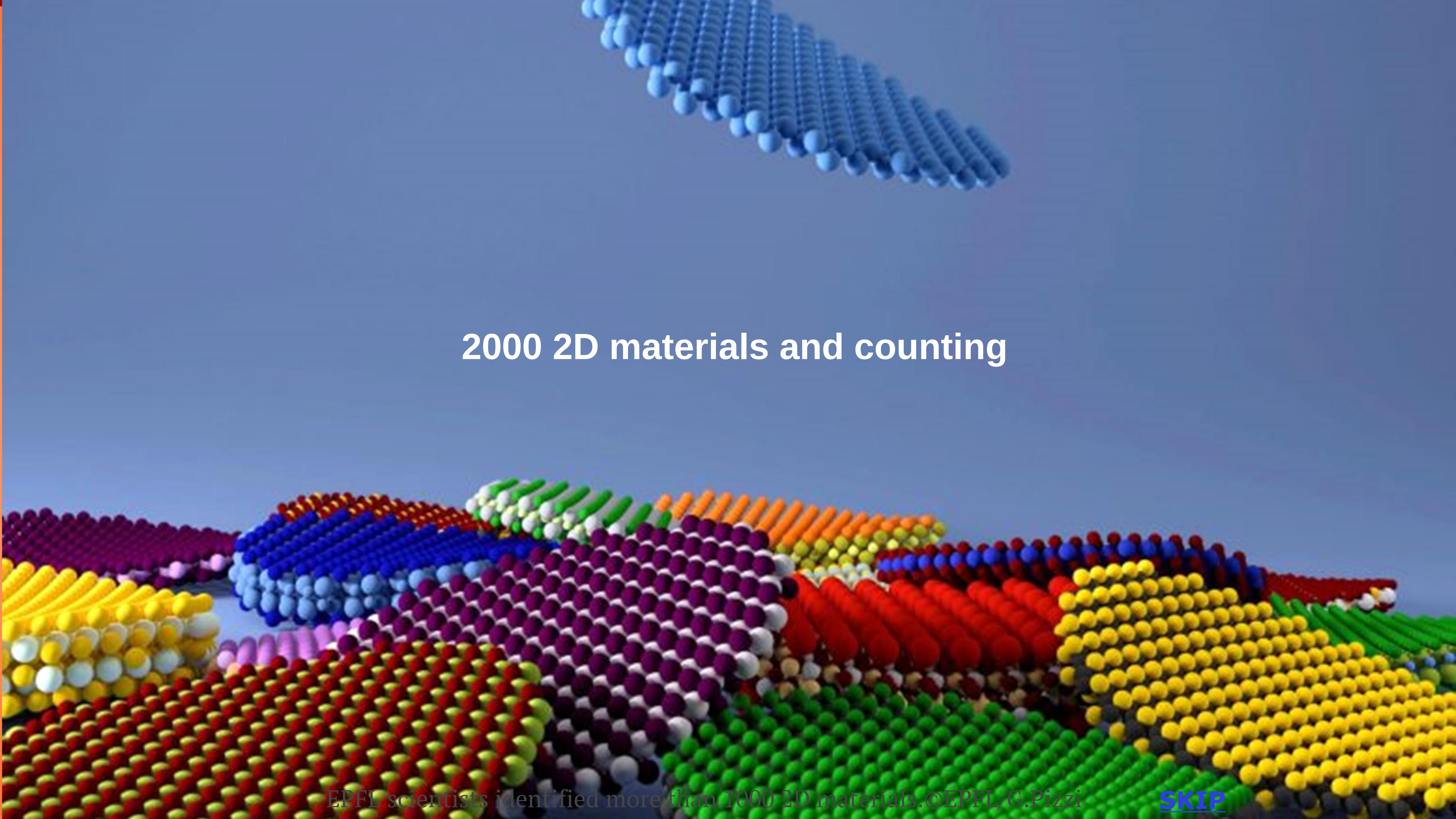


$\lambda_{m,1} = 10.2\,\text{nm}$ and $\lambda_{m,2} = 17.2\ \text{nm} \approx \sqrt{3}\,\lambda_{m,1}$.

4. vdw epitaxy : up-scaling?



2000 2D materials and counting



EPFL scientists identified more than 1000 2D materials.©EPFL/G.Pizzi

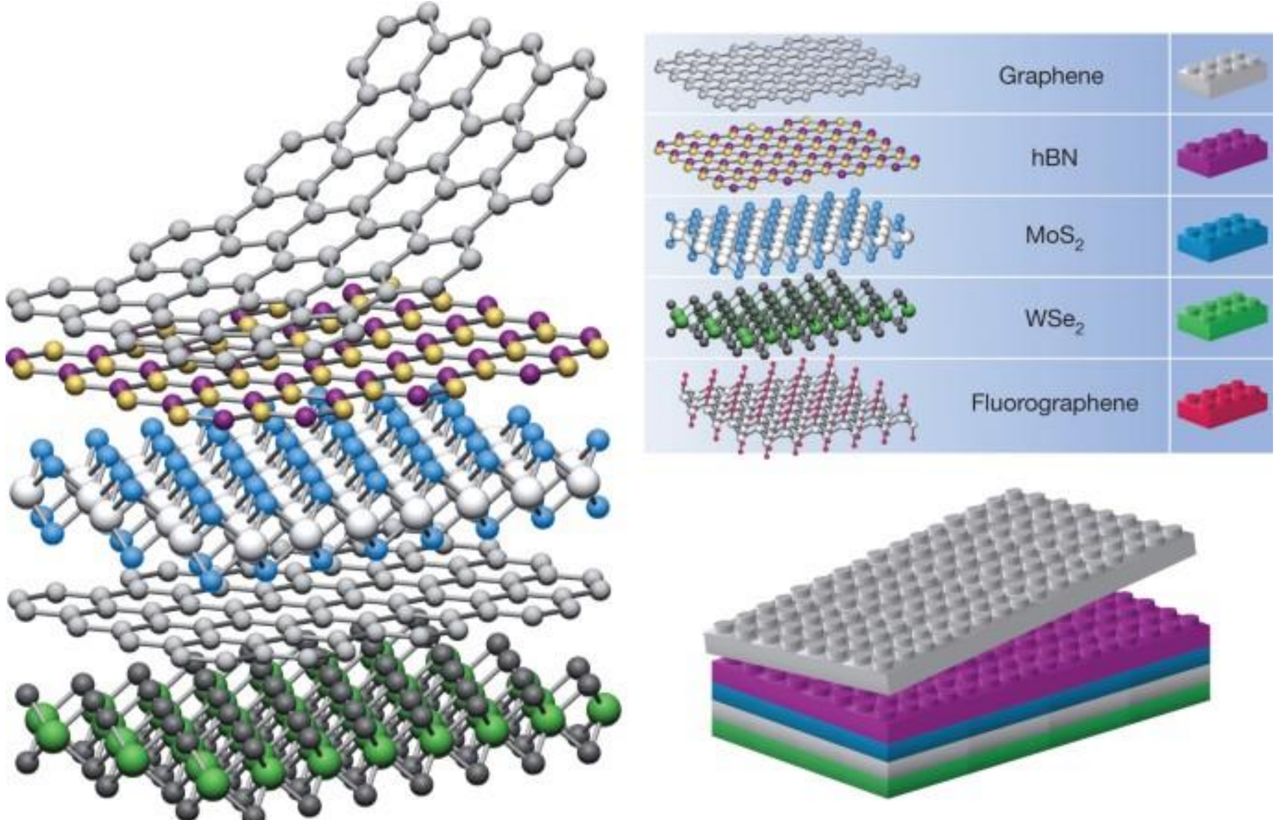
SKIP

25 JULY 2013 | VOL 499 | NATURE | 419

PERSPECTIVE

Van der Waals heterostructures

A. K. Geim[1,2] & I. V. Grigorieva[1]

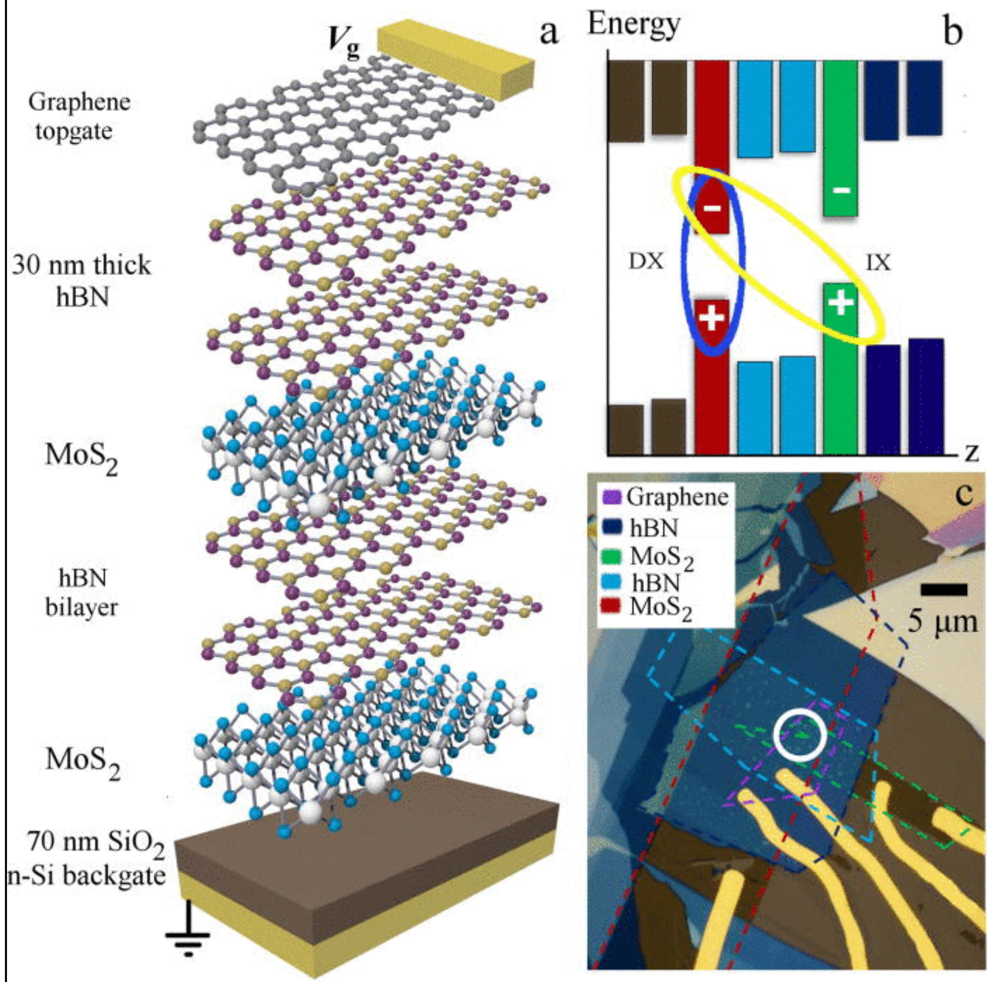


APPLIED PHYSICS LETTERS **108**, 101901 (2016)

CrossMark

Control of excitons in multi-layer van der Waals heterostructures

E. V. Calman,[1,a)] C. J. Dorow,[1] M. M. Fogler,[1] L. V. Butov,[1] S. Hu,[2] A. Mishchenko,[2] and A. K. Geim[2]
[1]*Department of Physics, University of California at San Diego, La Jolla, California 92093-0319, USA*
[2]*School of Physics and Astronomy, University of Manchester, Manchester M13 9PL, United Kingdom*



DTU

C2DB

The Computational 2D Materials Database

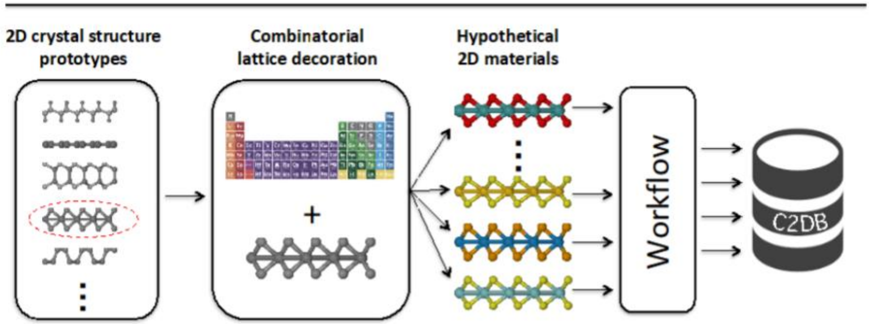
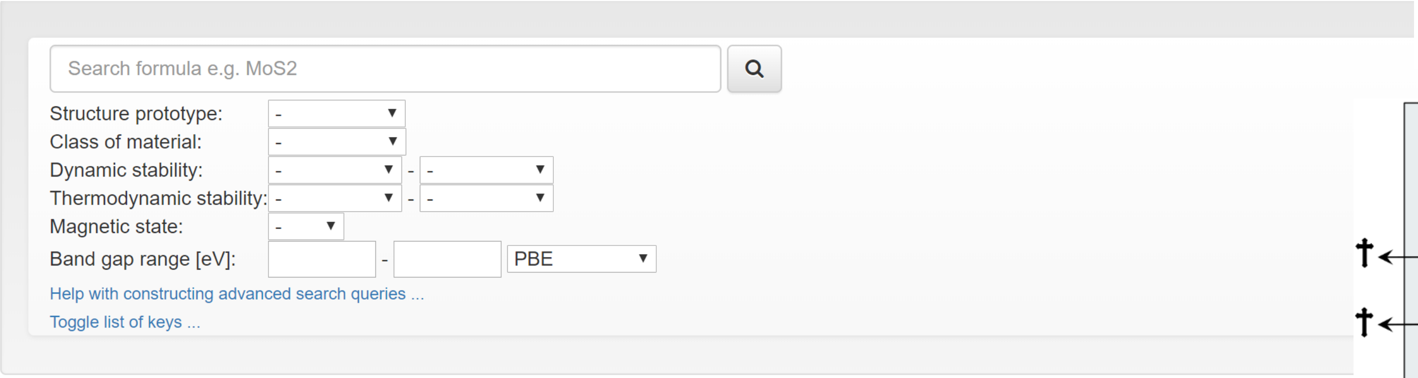
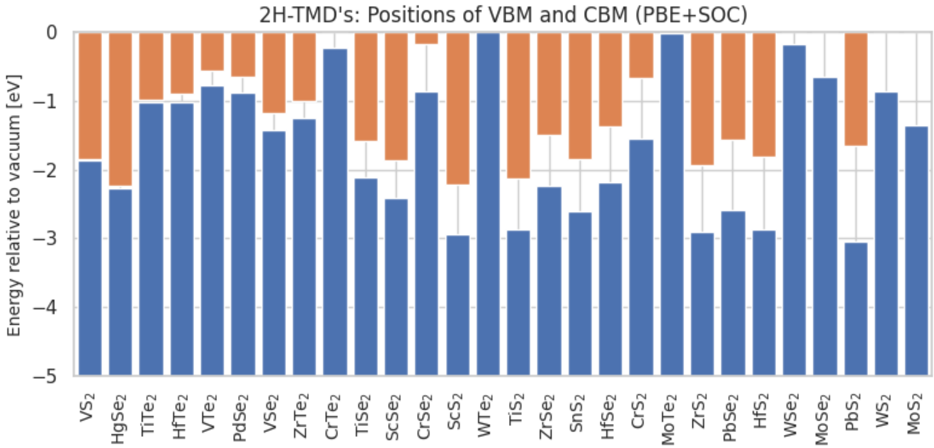
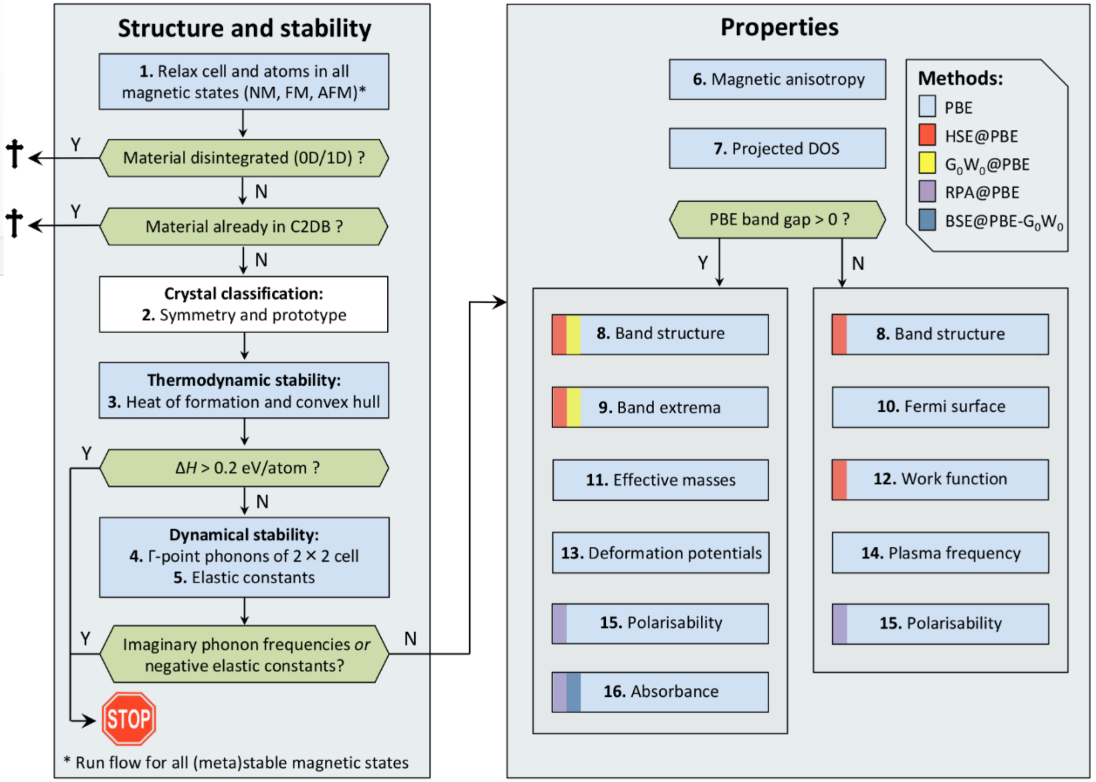
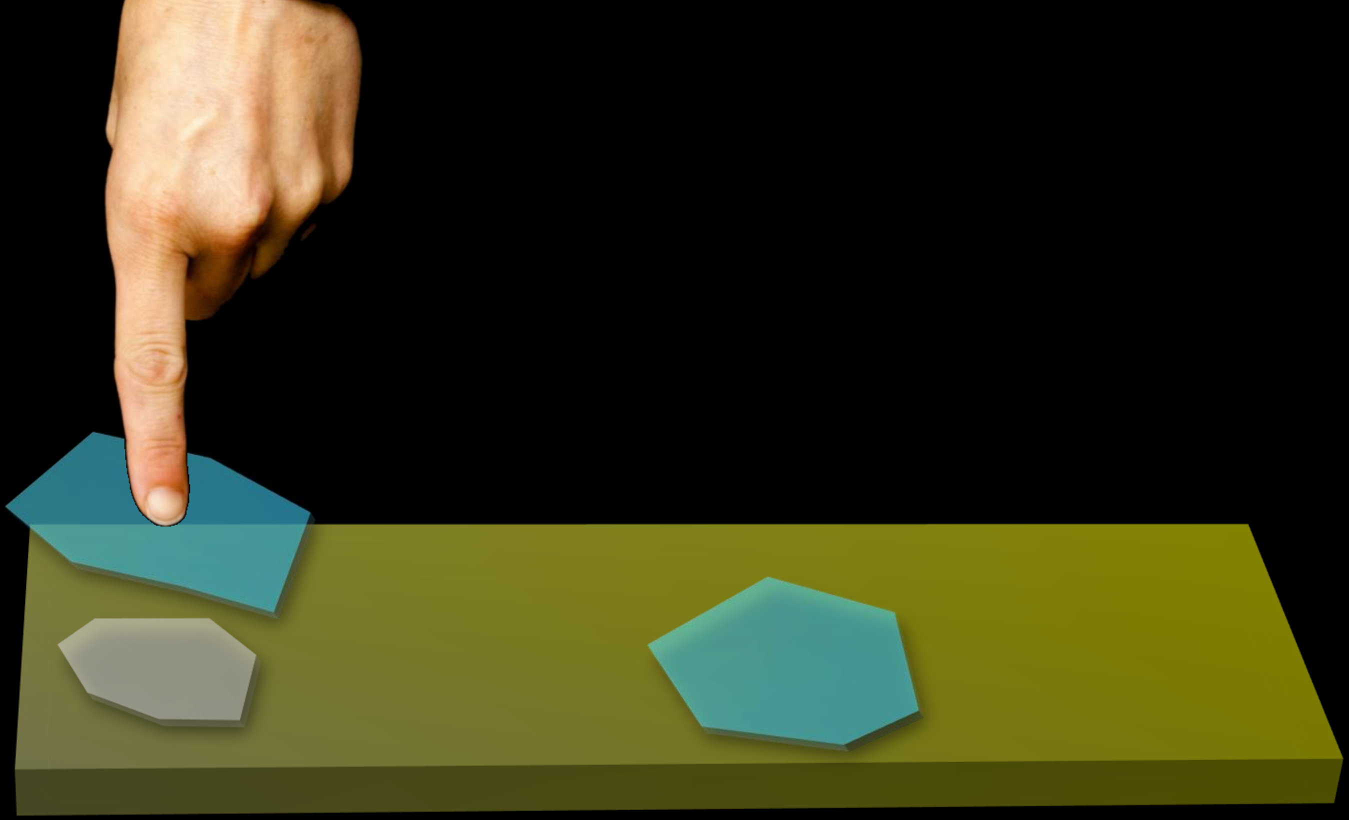


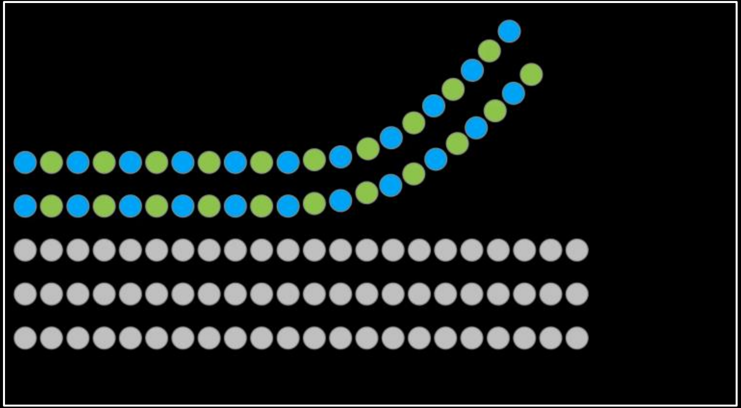
Figure 2. The materials in the C2DB are initially generated by decorating an experimentally known crystal structure prototype with atoms chosen from a (chemically reasonable) subset of the periodic table.

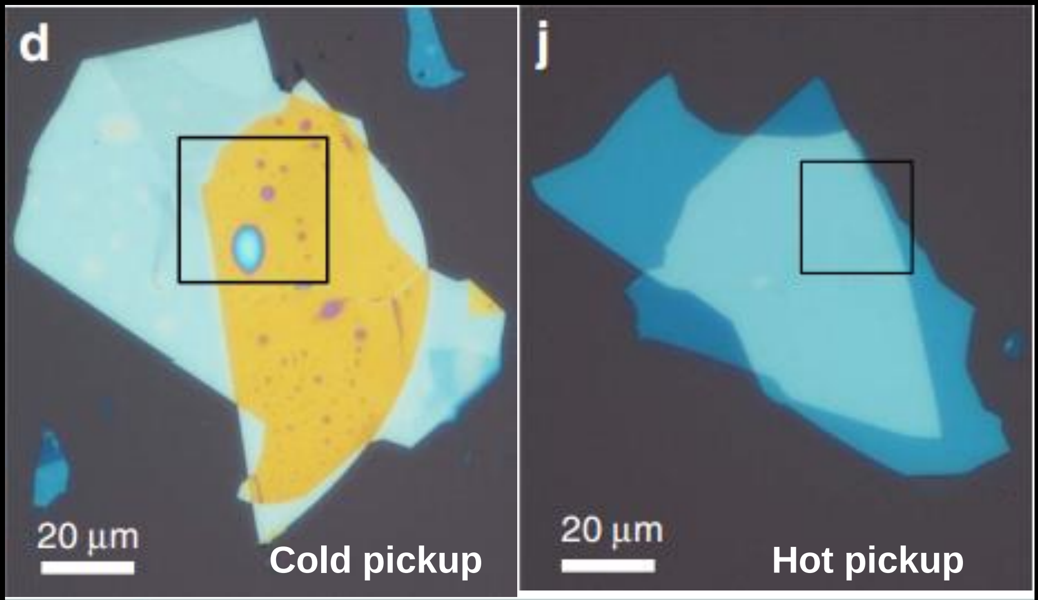












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ARTICLE

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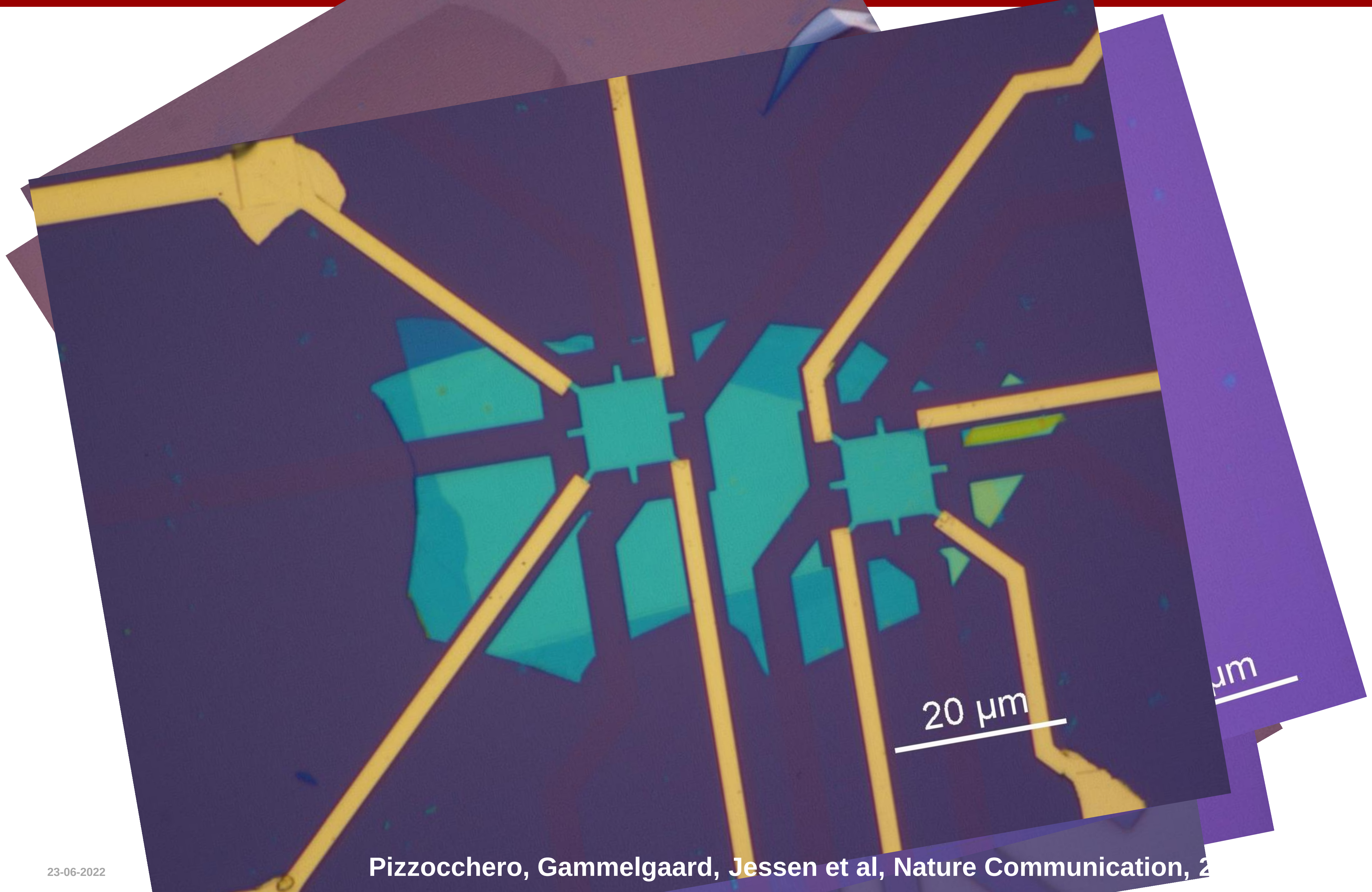
The hot pick-up technique for batch assembly of van der Waals heterostructures

Filippo Pizzocchero[1], Lene Gammelgaard[1], Bjarke S. Jessen[1], José M. Caridad[1], Lei Wang[2], James Hone[3], Peter Bøggild[1] & Timothy J. Booth[1]

The assembly of individual two-dimensional materials into van der Waals heterostructures enables the construction of layered three-dimensional materials with desirable electronic and optical properties. A core problem in the fabrication of these structures is the formation of clean interfaces between the individual two-dimensional materials which would affect device performance. We present here a technique for the rapid batch fabrication of van der Waals heterostructures, demonstrated by the controlled production of 22 mono-, bi- and trilayer graphene stacks encapsulated in hexagonal boron nitride with close to 100% yield. For the monolayer devices, we found semiclassical mean-free paths up to 0.9 μm, with the narrowest samples showing clear indications of the transport being affected by boundary scattering. The presented method readily lends itself to fabrication of van der Waals heterostructures in both ambient and controlled atmospheres, while the ability to assemble pre-patterned layers



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LETTERS

https://doi.org/10.1038/s41565-021-01061-5

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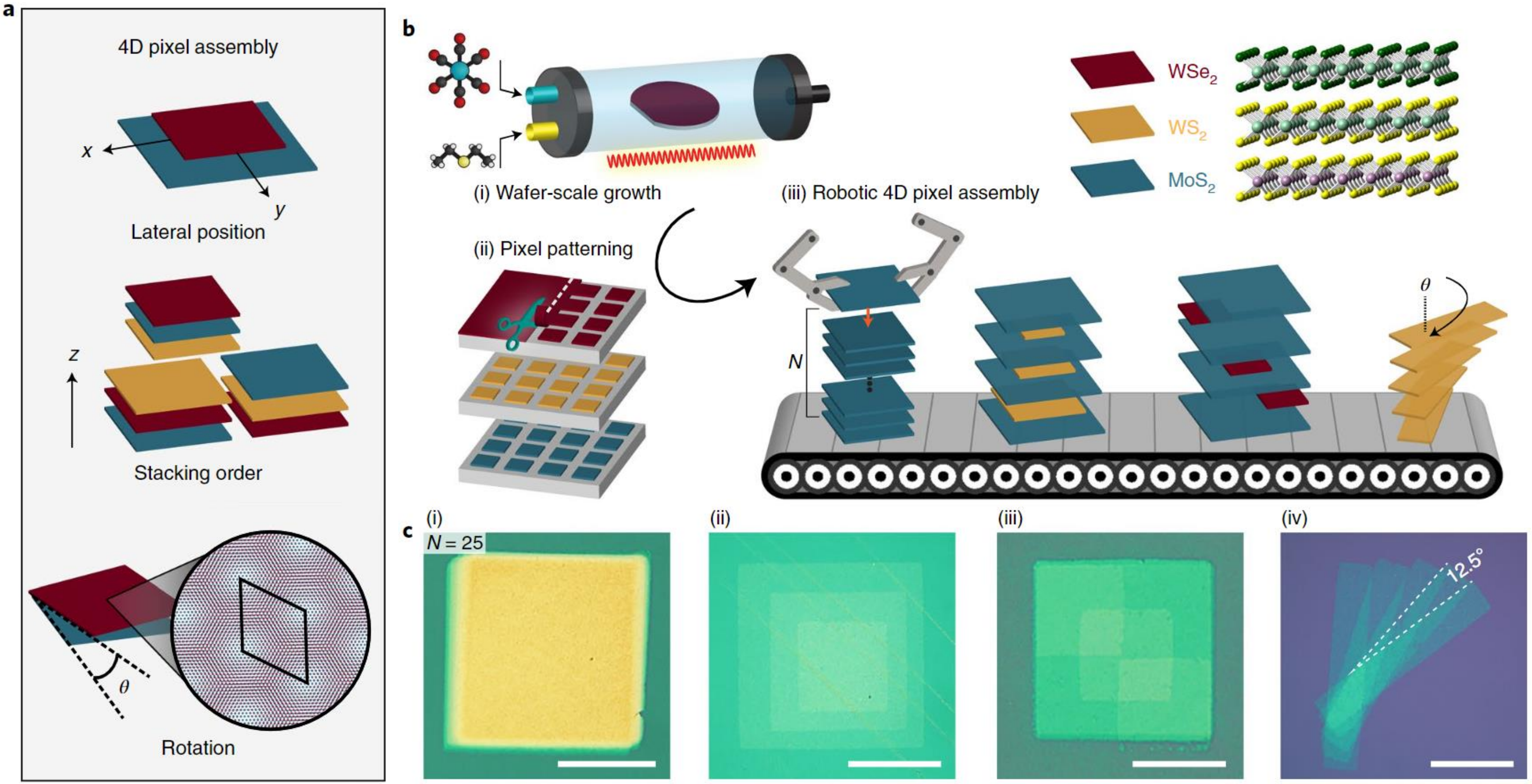
Robotic four-dimensional pixel assembly of van der Waals solids

Andrew J. Mannix[1,9,10], Andrew Ye[2,10], Suk Hyun Sung[3], Ariana Ray[4], Fauzia Mujid[5], Chibeom Park[5], Myungjae Lee[1], Jong-Hoon Kang[5], Robert Shreiner[6], Alexander A. High[2,7], David A. Muller[4,8], Robert Hovden[3] and Jiwoong Park[1,2,5] ✉



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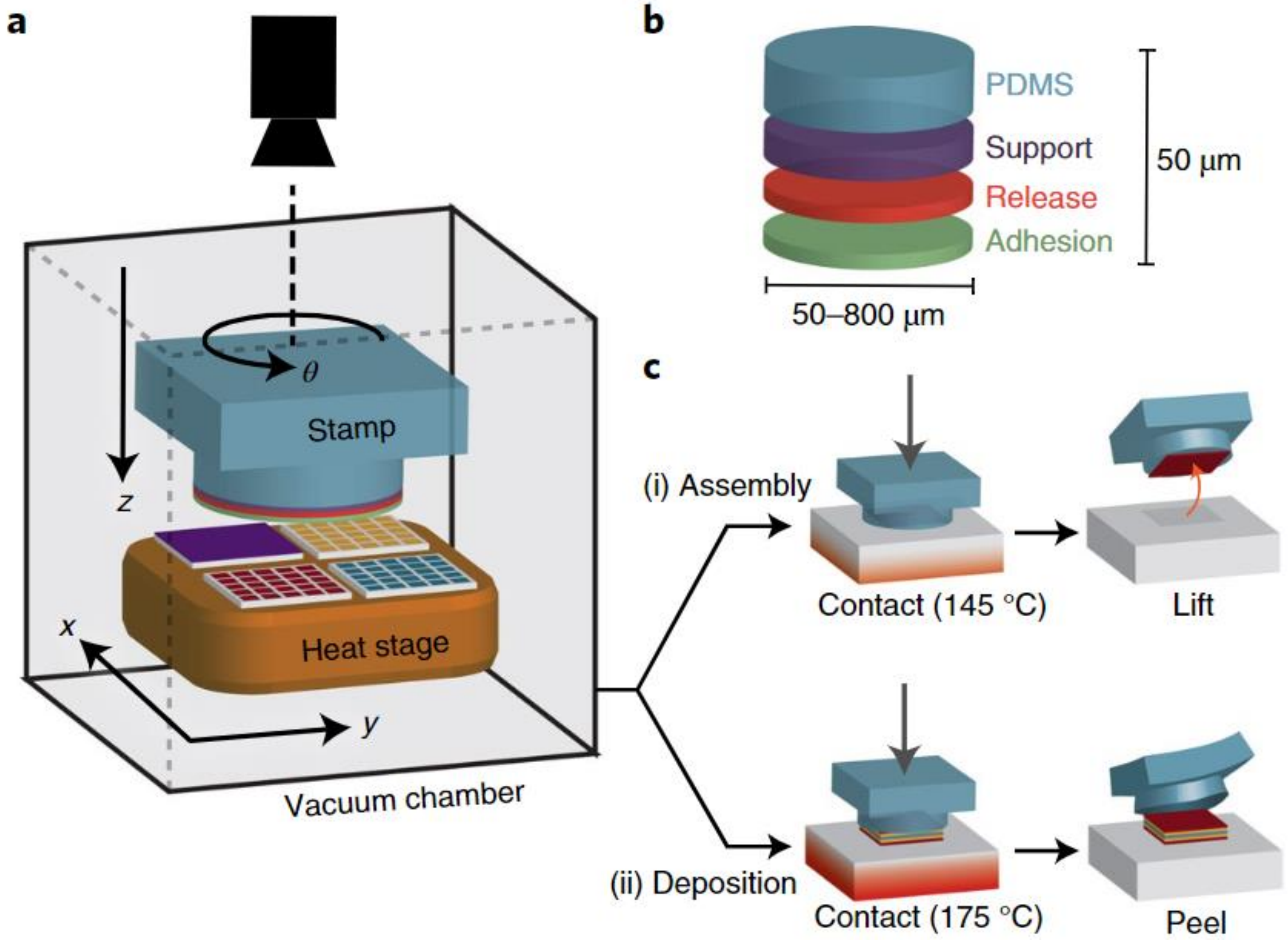

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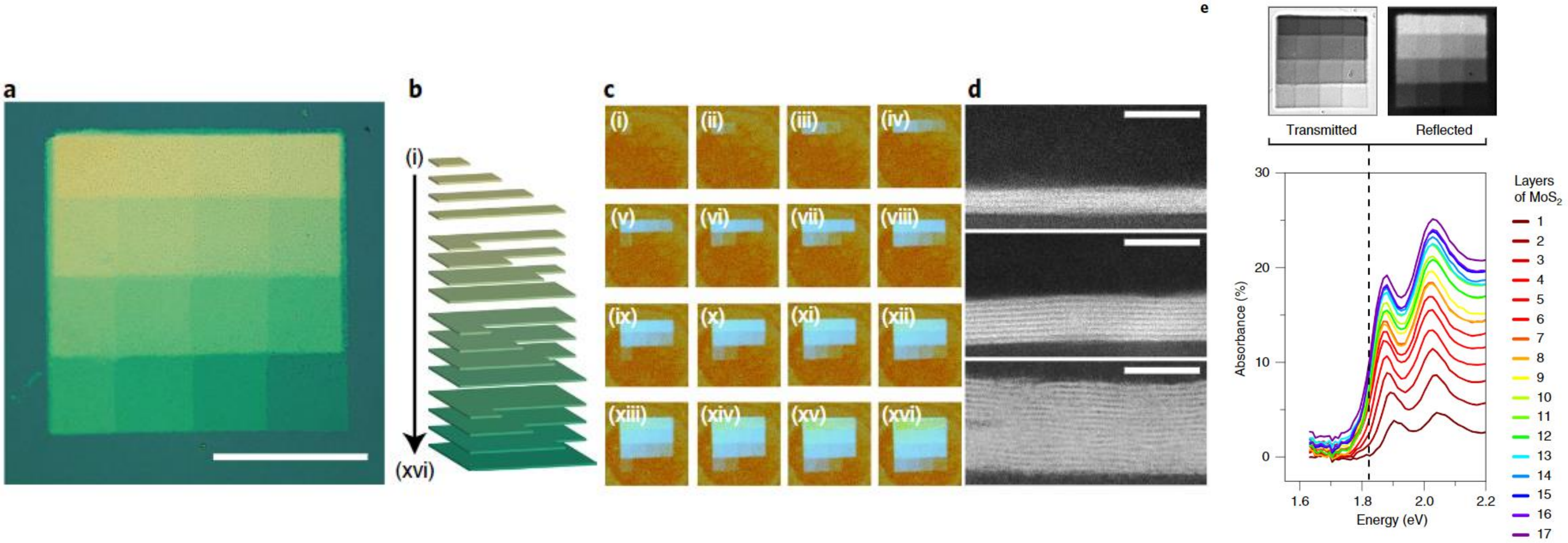
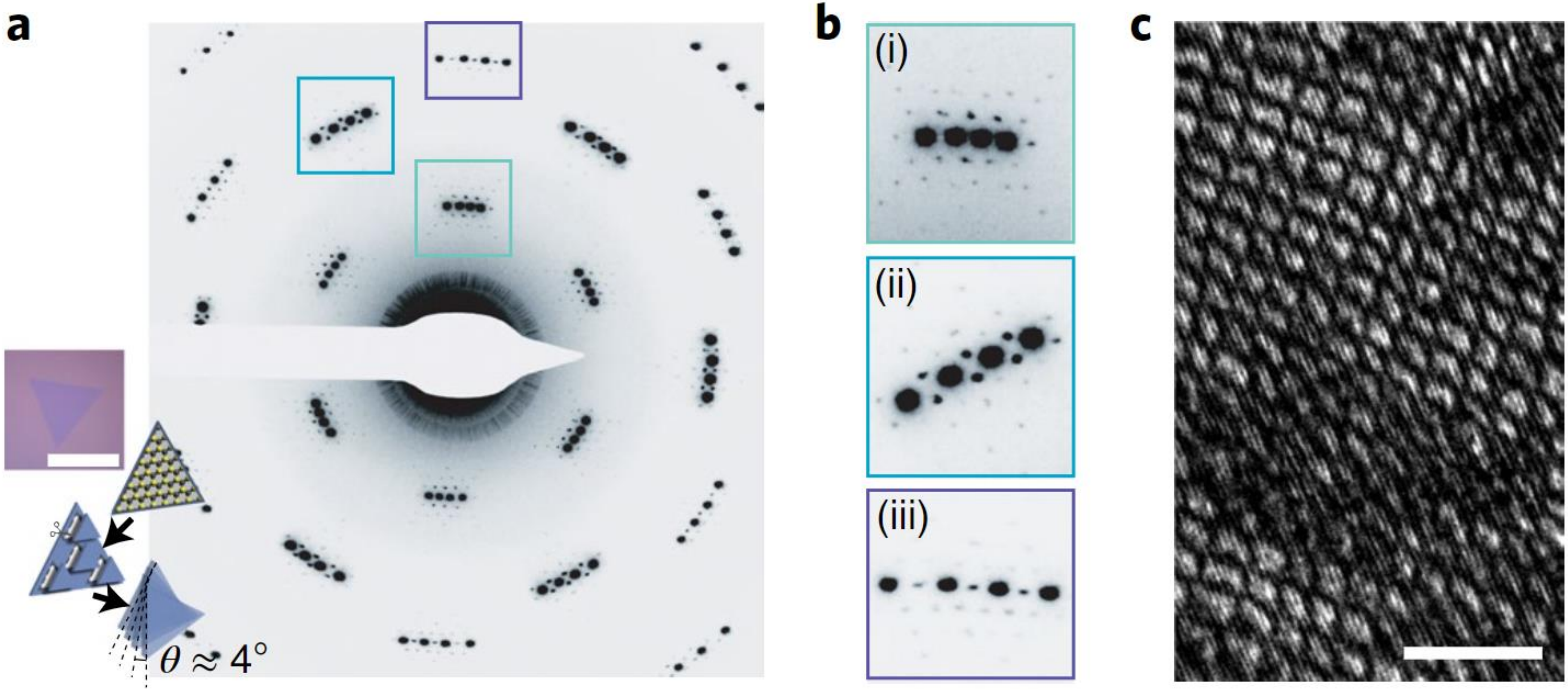
Optical assay of N-layer stacked MoS2



https://doi.org/10.1038/s41565-021-01061-5

Controlled angular epitaxy



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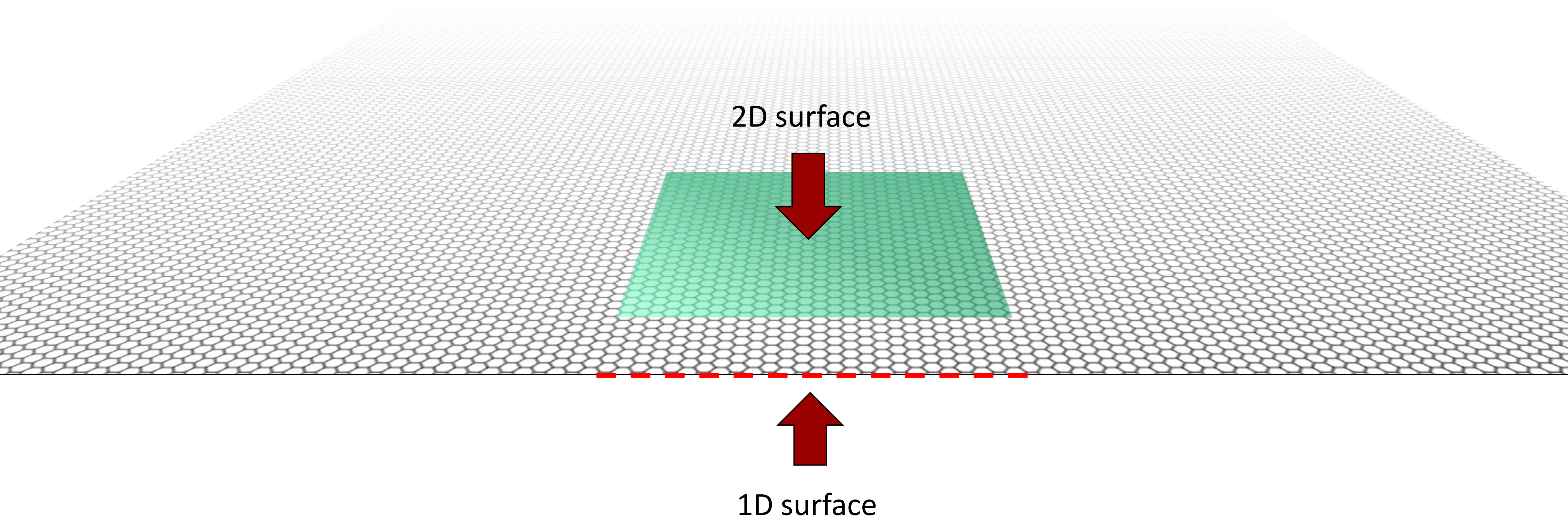
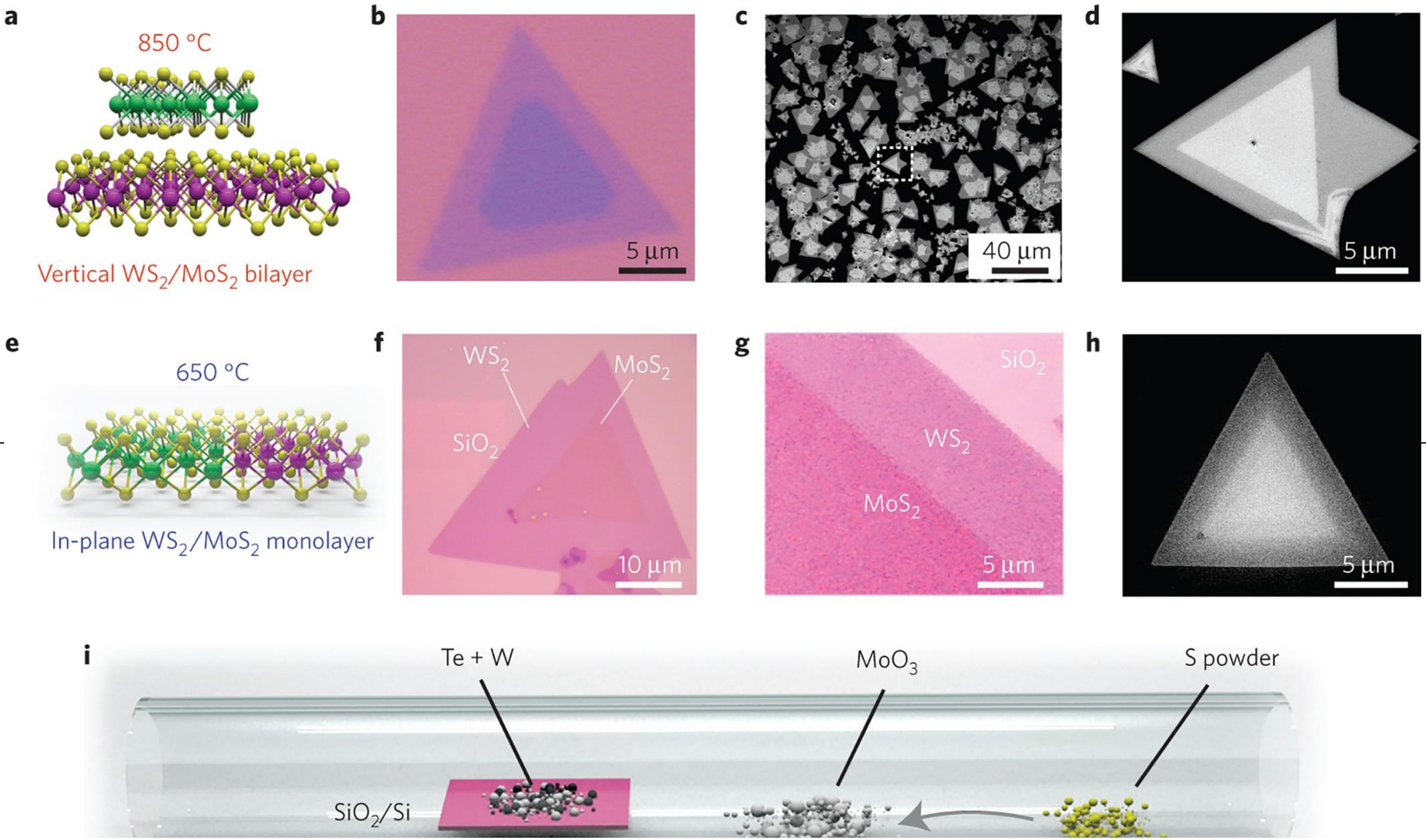


In a 2D material the bulk is a surface, and the surface is an edge



Nature Materials **volume 13**, pages1135–1142 (2014)

Engineering vdW epitaxy:

materials?
Modelling?
Patterning?
Upscaling?
Applications?