How can simple models help us understand experiments?

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Scientific Computing Laboratory
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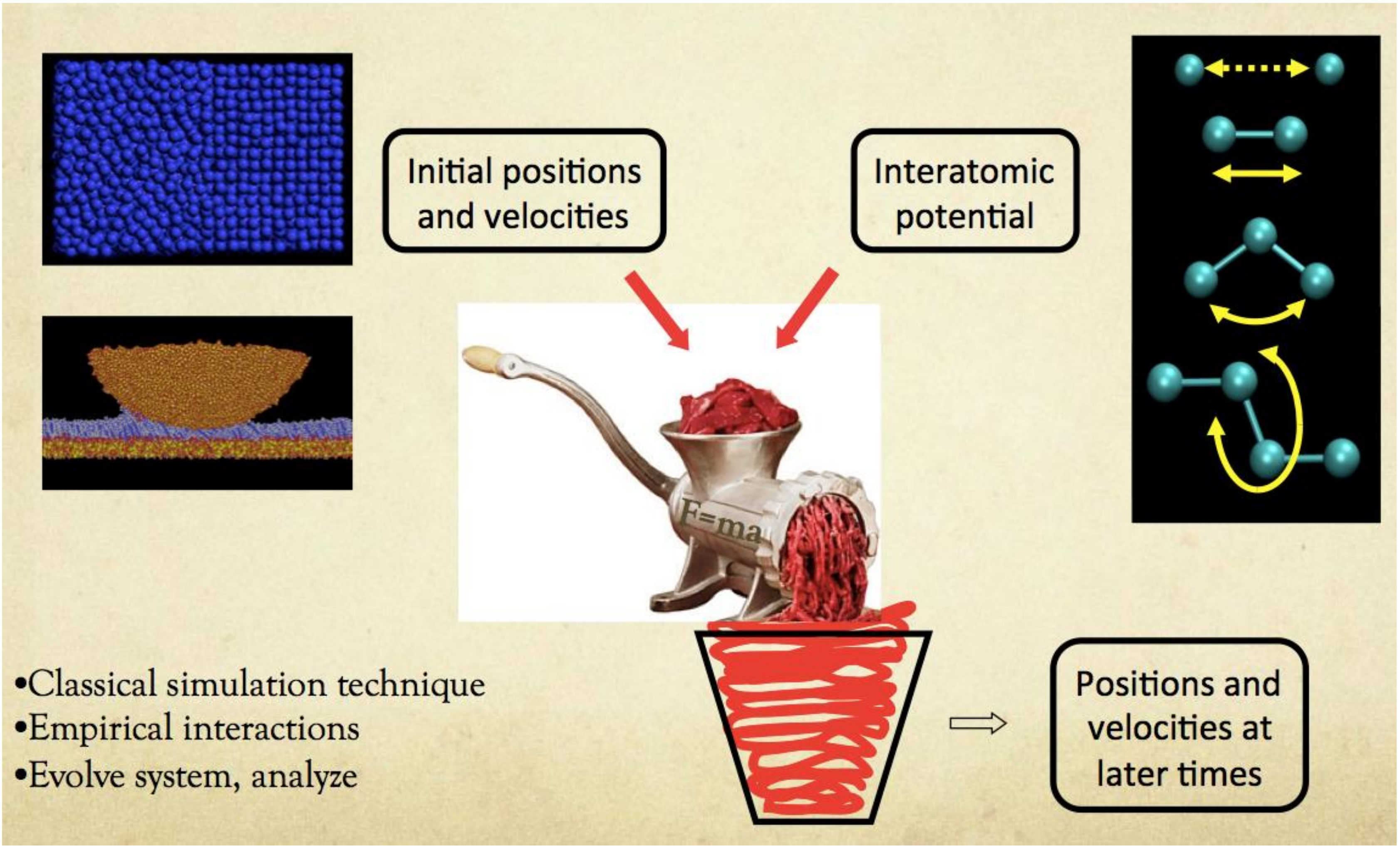
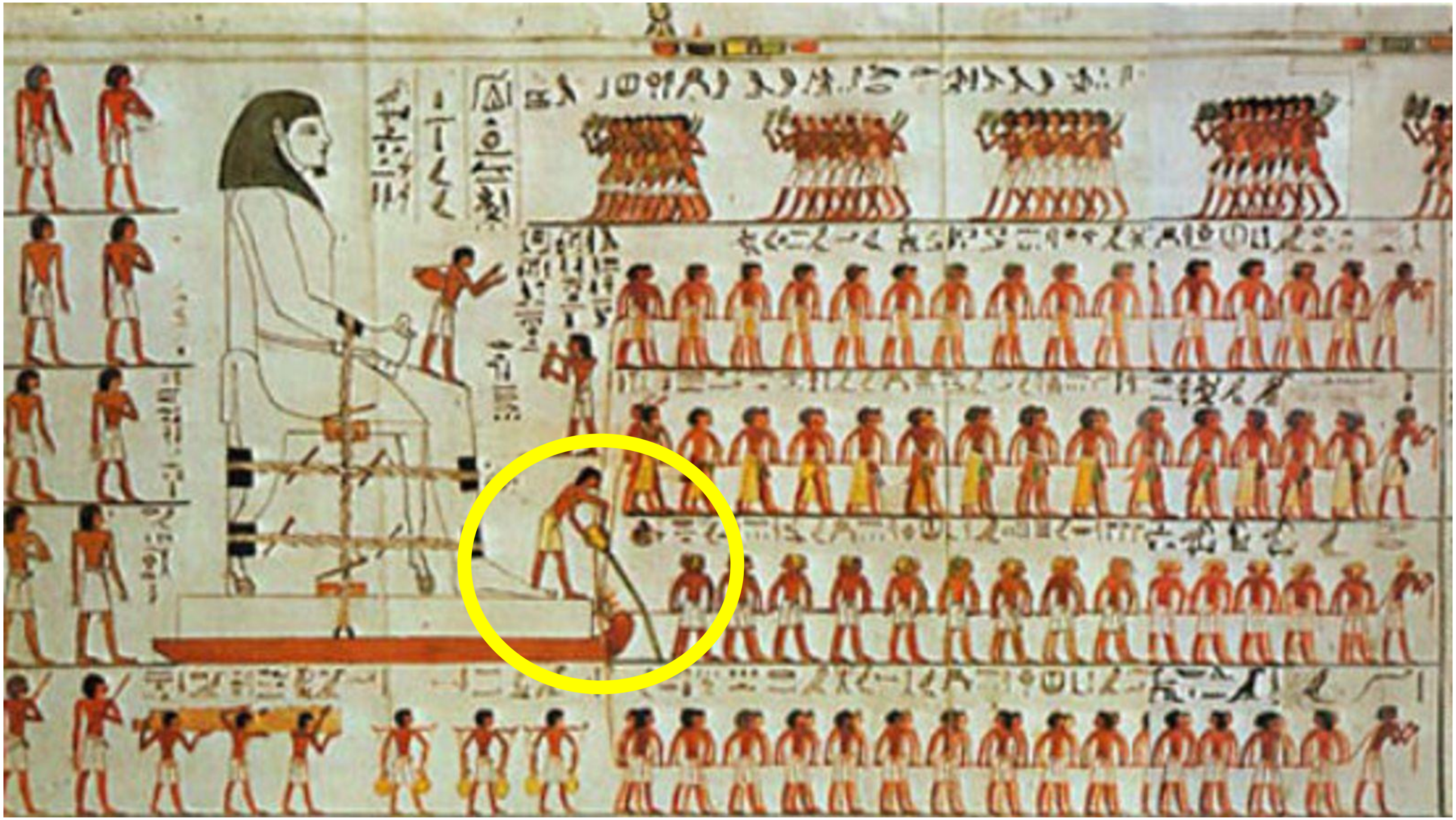
How much “simple” is simple?



Plan of lecture

- A brief history of tribology
- Modeling of AFM experiments
- Coarse grainded models of ionic liquids
- Magnetic cubes
- Future (water, scale trancending systems)

A brief history of tribology :
quest for controlled experiment



A brief history of tribology :

Early history (three laws):

Law of Leonardo (da Vinci):
Friction is independent on the area of contact.

Law of Euler and Amontons:
Friciton is proportional to the loading force.

Law of Coulomb:
Friction is independent on the velocity.

History of tribology :

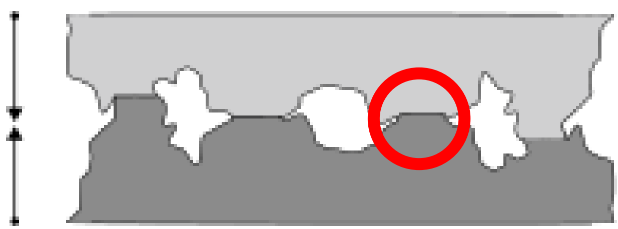
‘50 F. P. Bowden and D. Tabor

B&T model assumes that friction is proportional to both the real area of contact and a mean lateral force per unit area, the so-called shear strength.

<u>Contact area is approximately 1% of visible area!</u>

History of tribology :

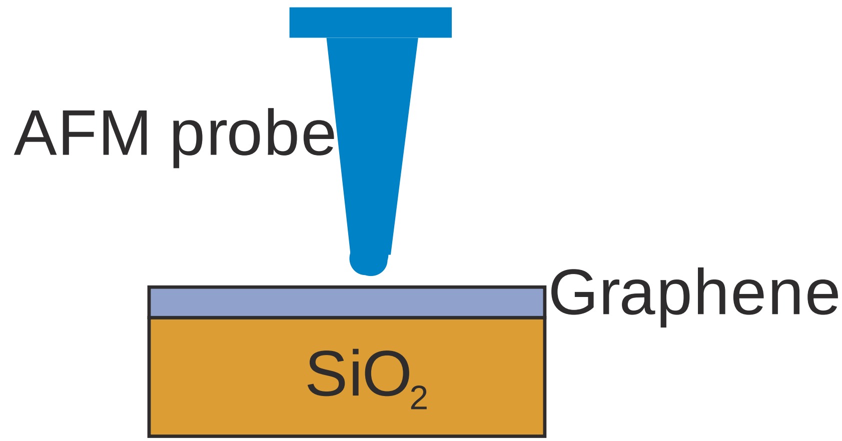
F. P. Bowden and D. Tabor –
Hertzian elastic theory
non-linear friction-load dependence $F \sim (L^*)^{2/3}$
but load on single asperity $L^* \sim L^{3/2}$



'90 We could prove
F. P. Bowden and D. Tabor law with
atomic force microscope (AFM) and
friction force microscope (FFM).

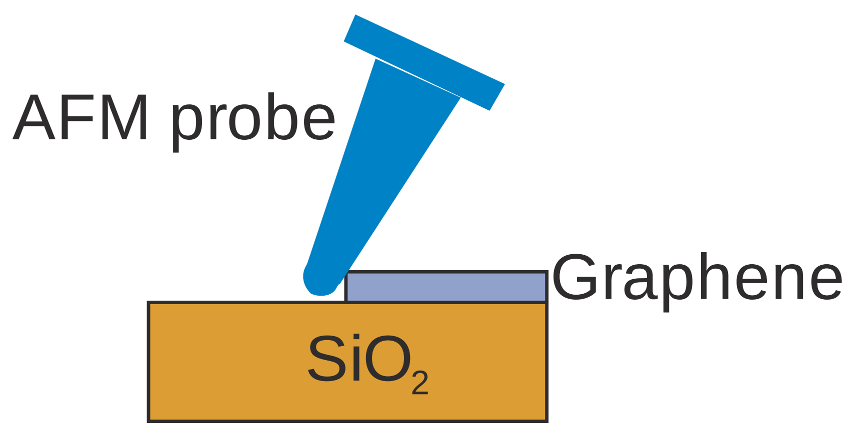
B. Vasic, A. Matkovic, R. Gajic, IS, Wear Properties of Graphene Edges Probed by Atomic Force Microscopy Based Lateral Manipulation, Carbon 107, 723 (2016).

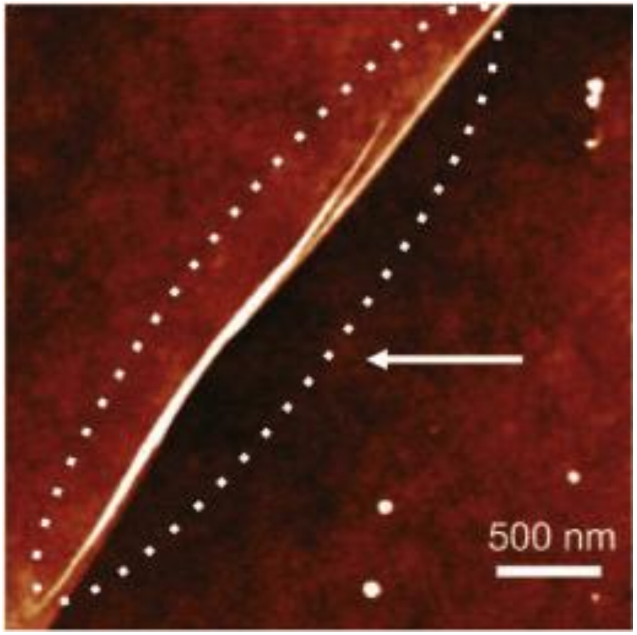
- So far, graphene mechanics was investigated by AFM probe **above graphene**!

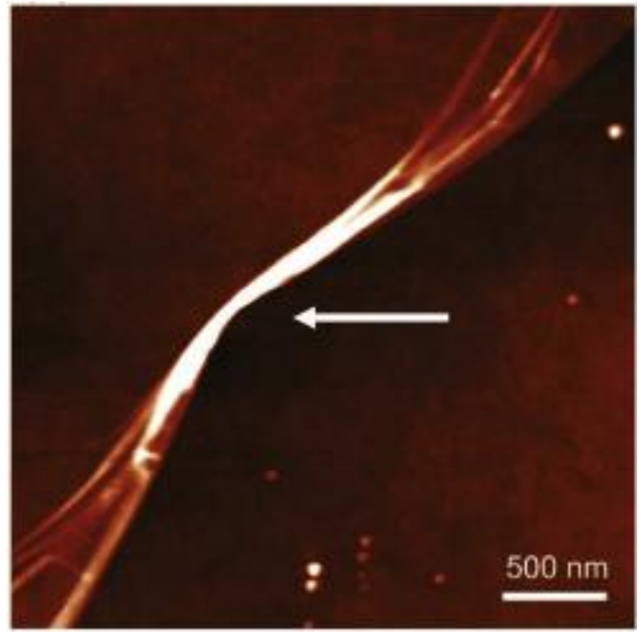


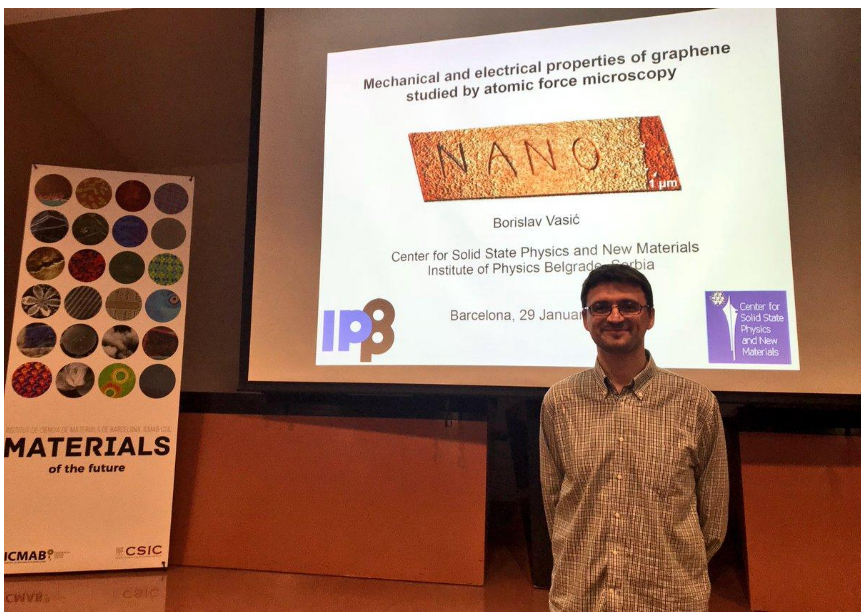
- Our aim:

  force applied on graphene edges - response of graphene flakes to **lateral forces**!

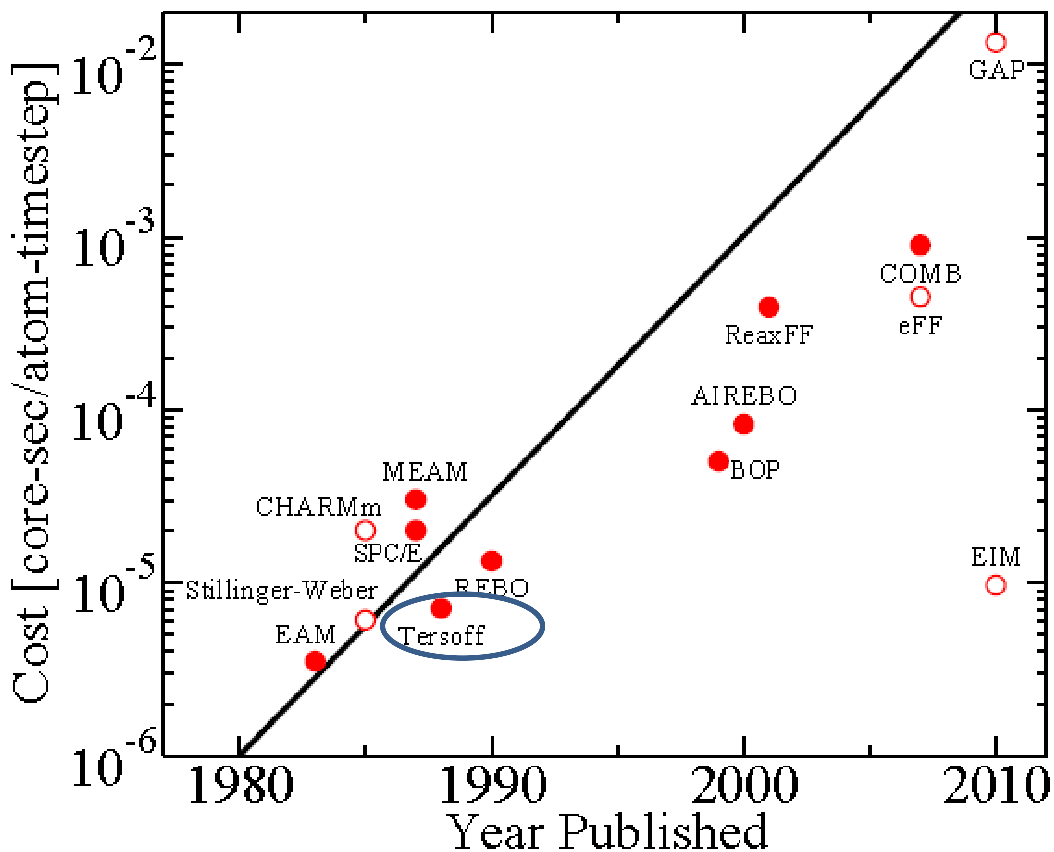



500 nm

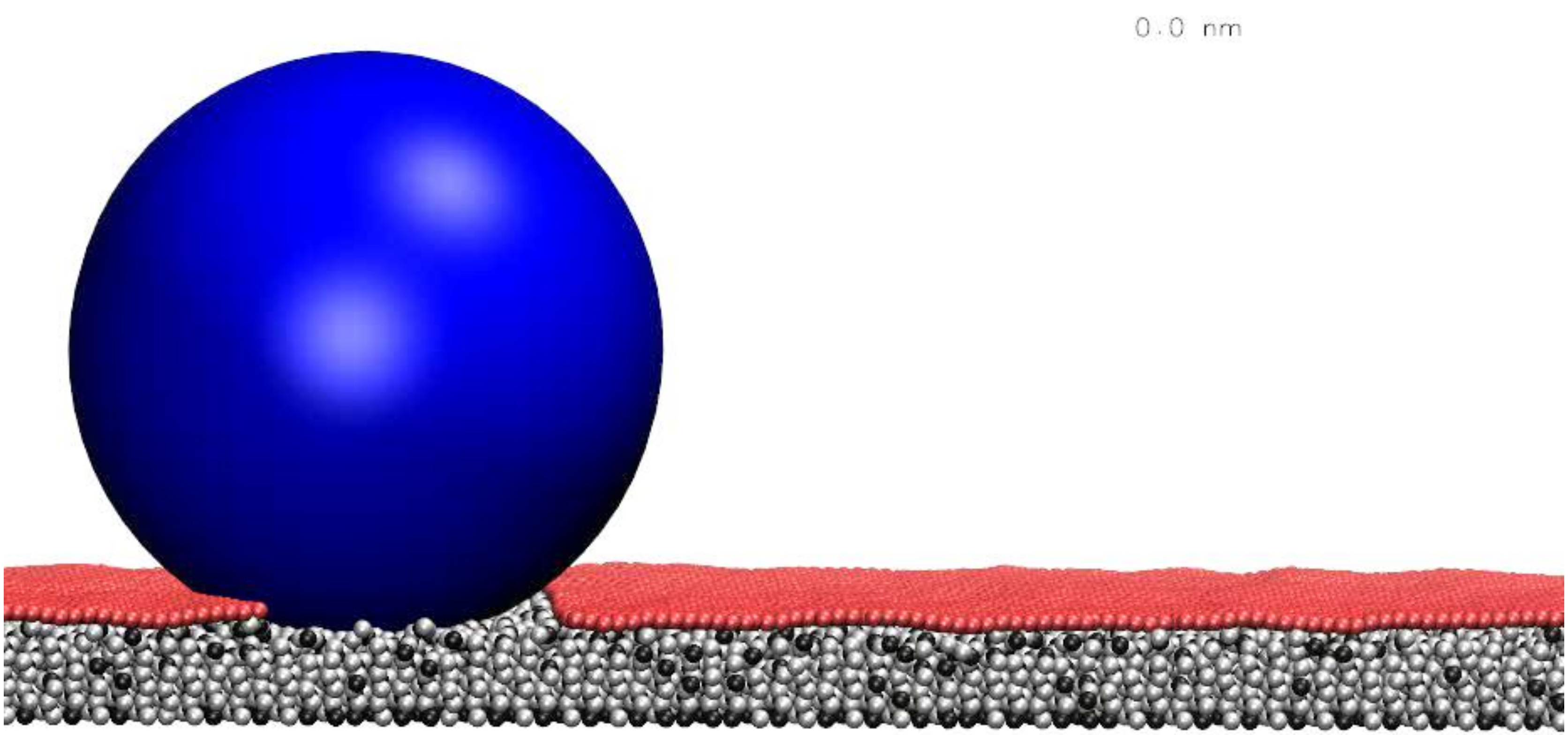

500 nm


Mechanical and electrical properties of graphene
studied by atomic force microscopy
NANO
1 µm
Borislav Vasić
Center for Solid State Physics and New Materials
Institute of Physics Belgrade
Barcelona, 29 Januar
Center for Solid State Physics and New Materials
MATERIALS
of the future
ICMAB
CSIC

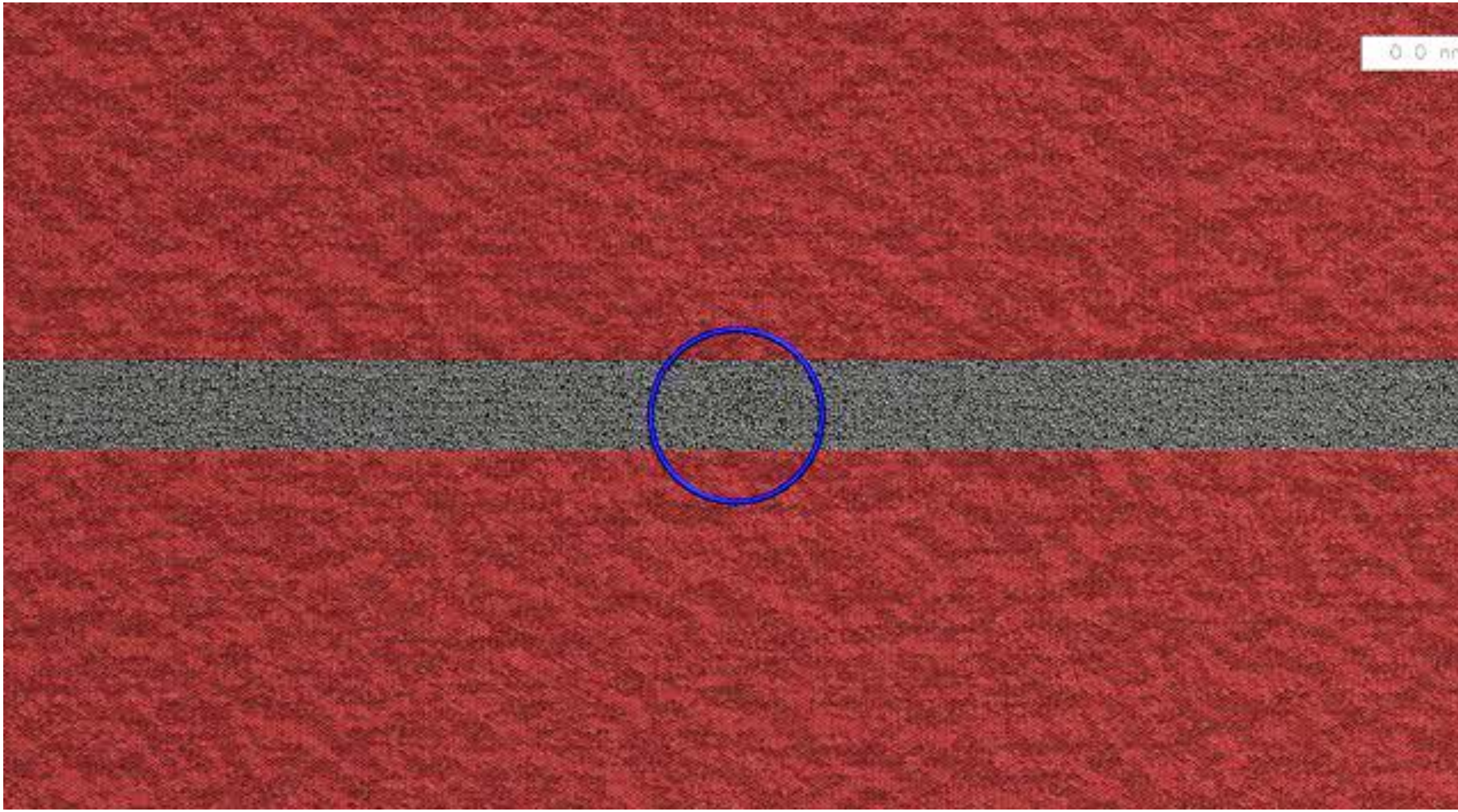
Simple model > big system

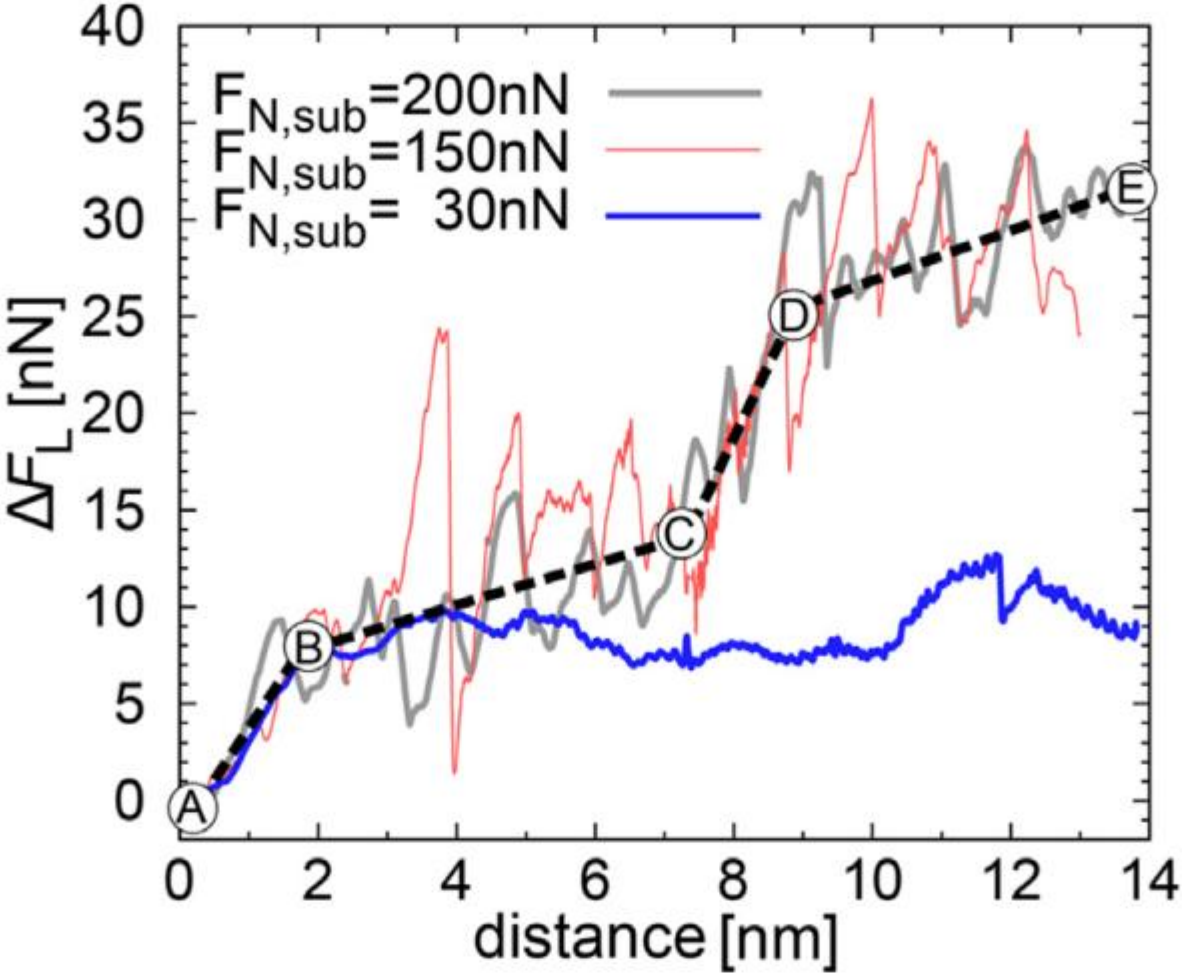


MD simulations



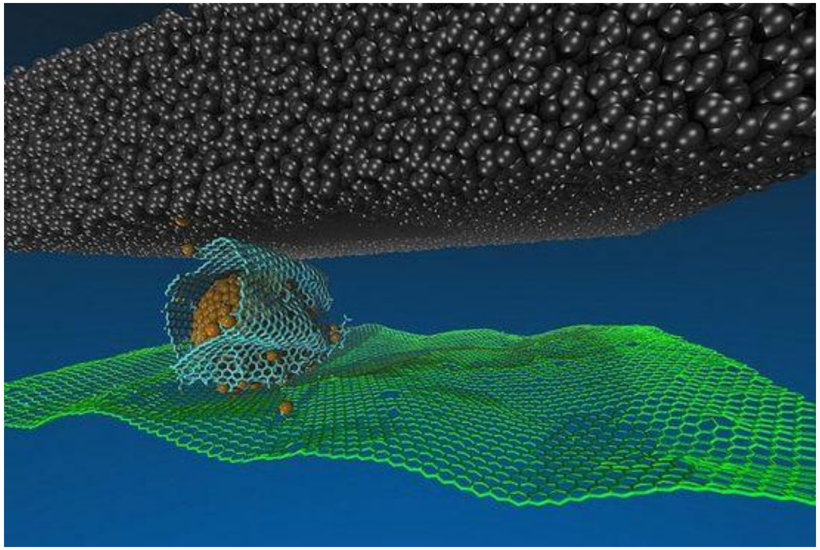
MD simulations

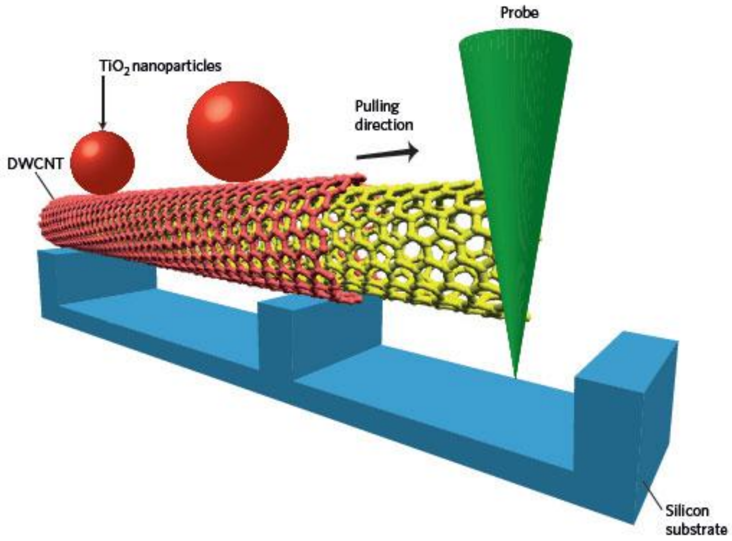




Wear properties of graphene edges probed by atomic force microscopy based lateral manipulation
B. Vasić, A. Matković, R. Gajić, I. S.
Carbon 107, 723-732 (2016)

Superlubricity for nanotech

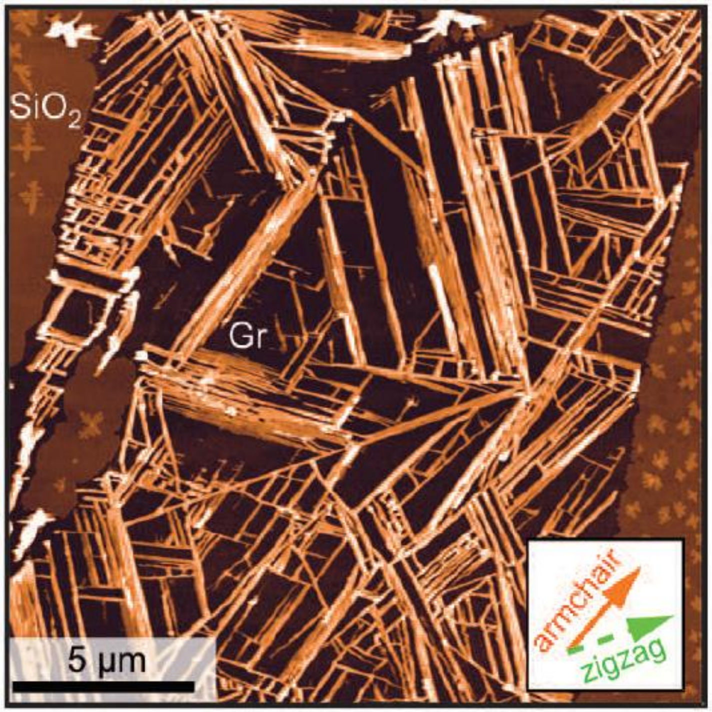


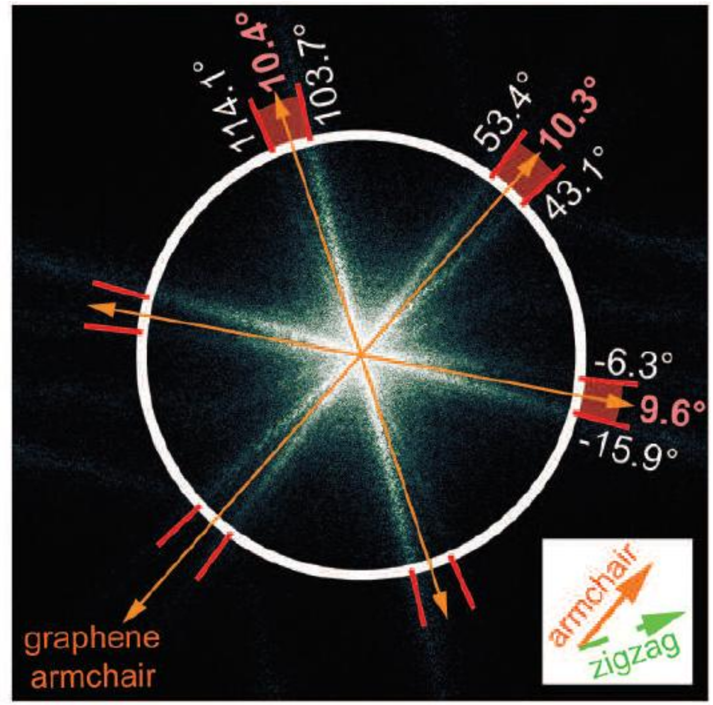


Macroscale superlubricity enabled by graphene nanoscroll formation
Diana Berman, Sanket A. Deshmukh, Subramanian K. R. S. Sankaranarayanan, Ali Erdemir, & Anirudha V. Sumant, *Science* 348, 1118-1122 (2015)

Superlubricity in centimetres-long double-walled carbon nanotubes under ambient conditions
Rufan Zhang, Zhiyuan Ning, Yingying Zhang, Quanshui Zheng, Qing Chen, Huanhuan Xie, Qiang Zhang, Weizhong Qian & Fei Wei
Nature Nanotechnology **8**, pages912–916 (2013)

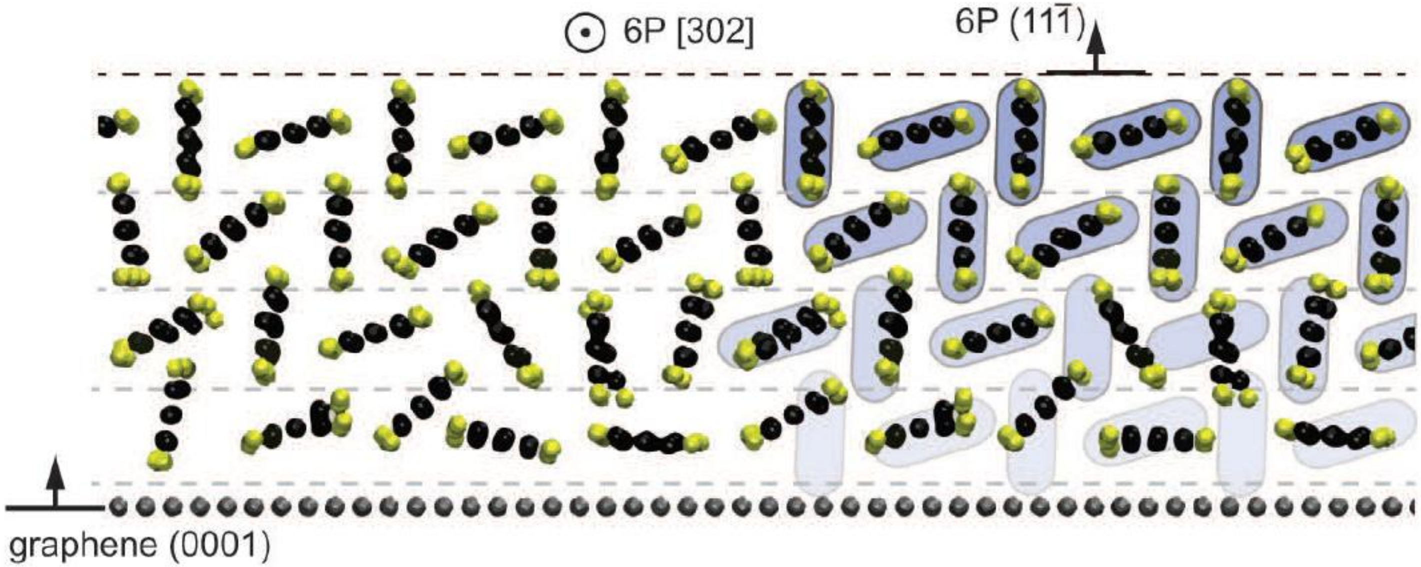
Organic crystals on graphene

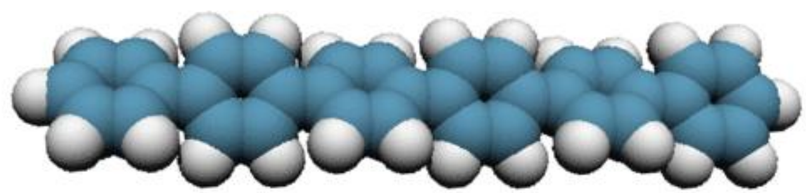


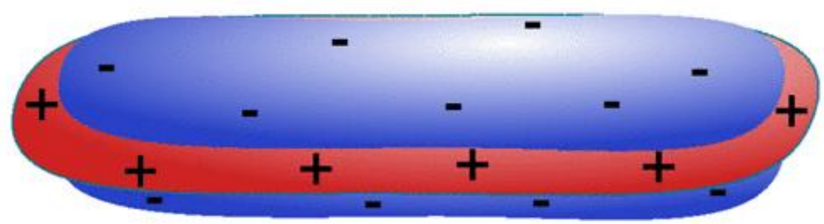


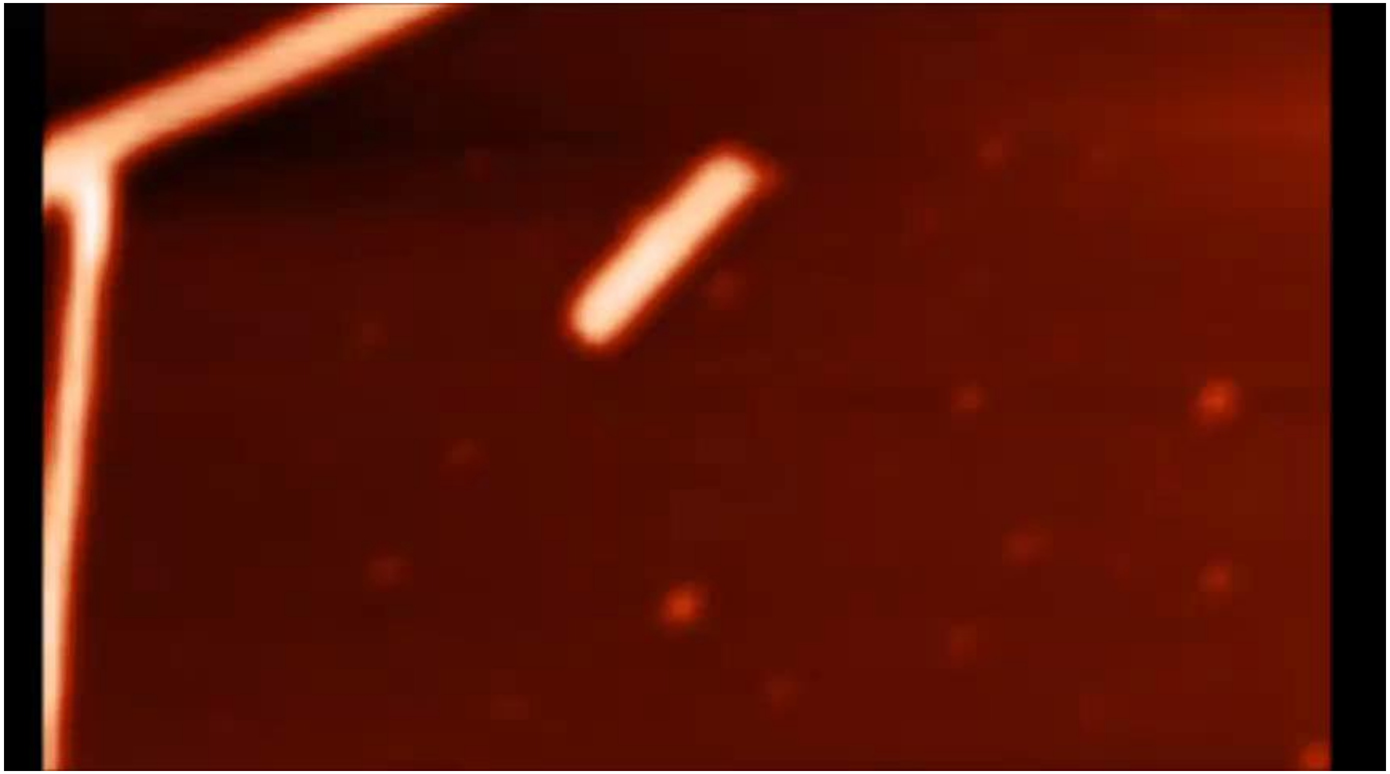
B. Vasić, IS, A. Matković, M. Kratzer, C. Ganser, R. Gajić, C. Teichert,
Molecules on rails: friction anisotropy and preferential sliding directions of organic nanocrystallites on two-dimensional materials
Nanoscale 10, 18835-18845 (2018).

Organic crystals on graphene

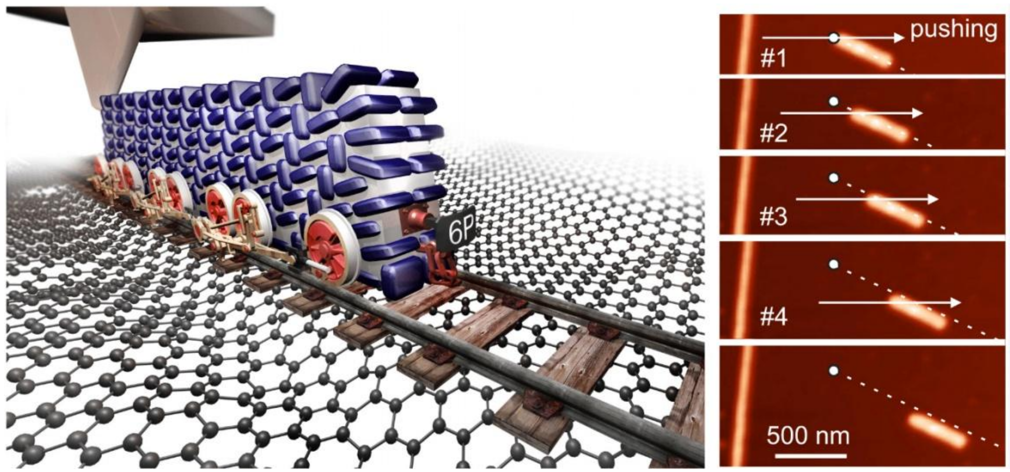


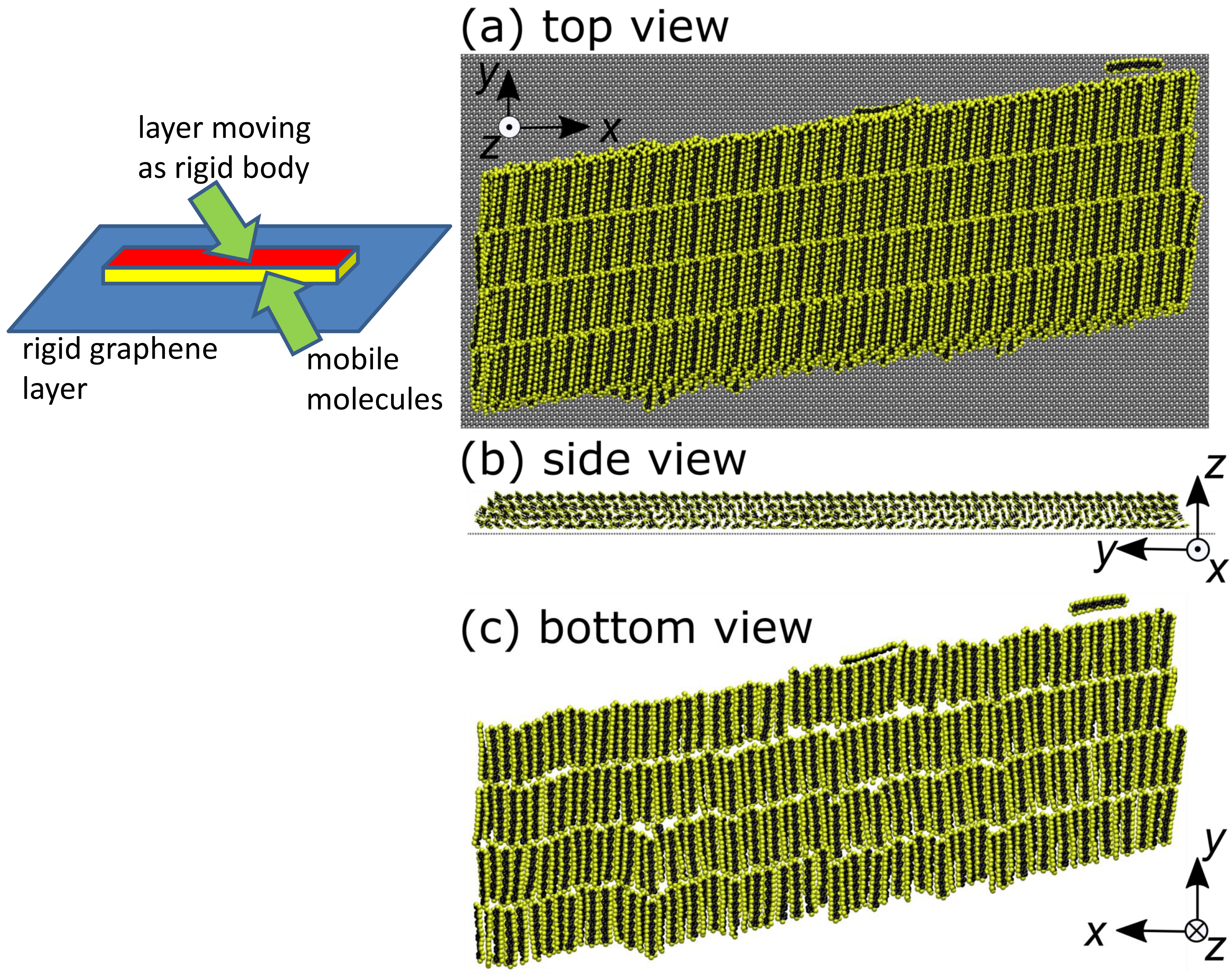




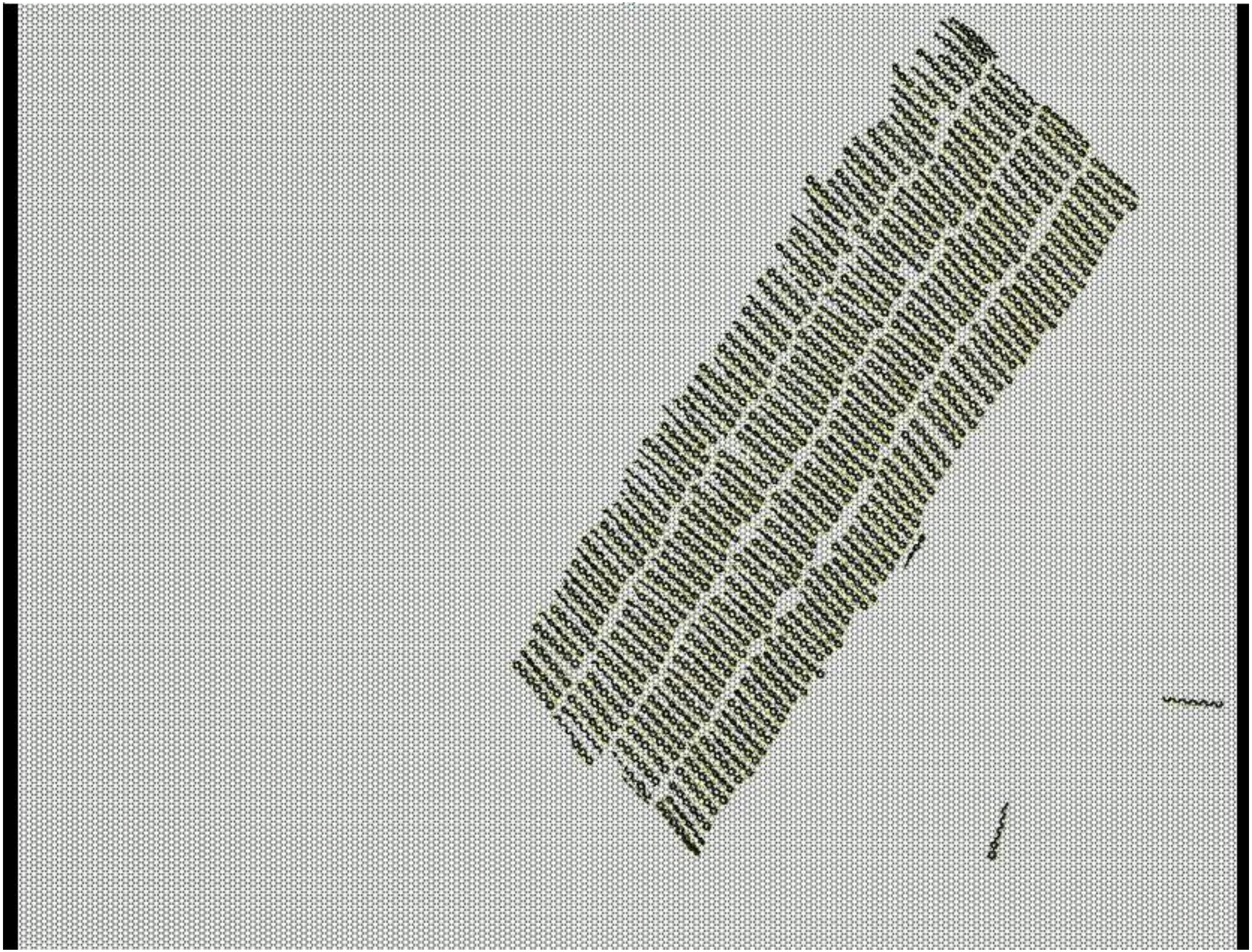


organic crystals on tracks

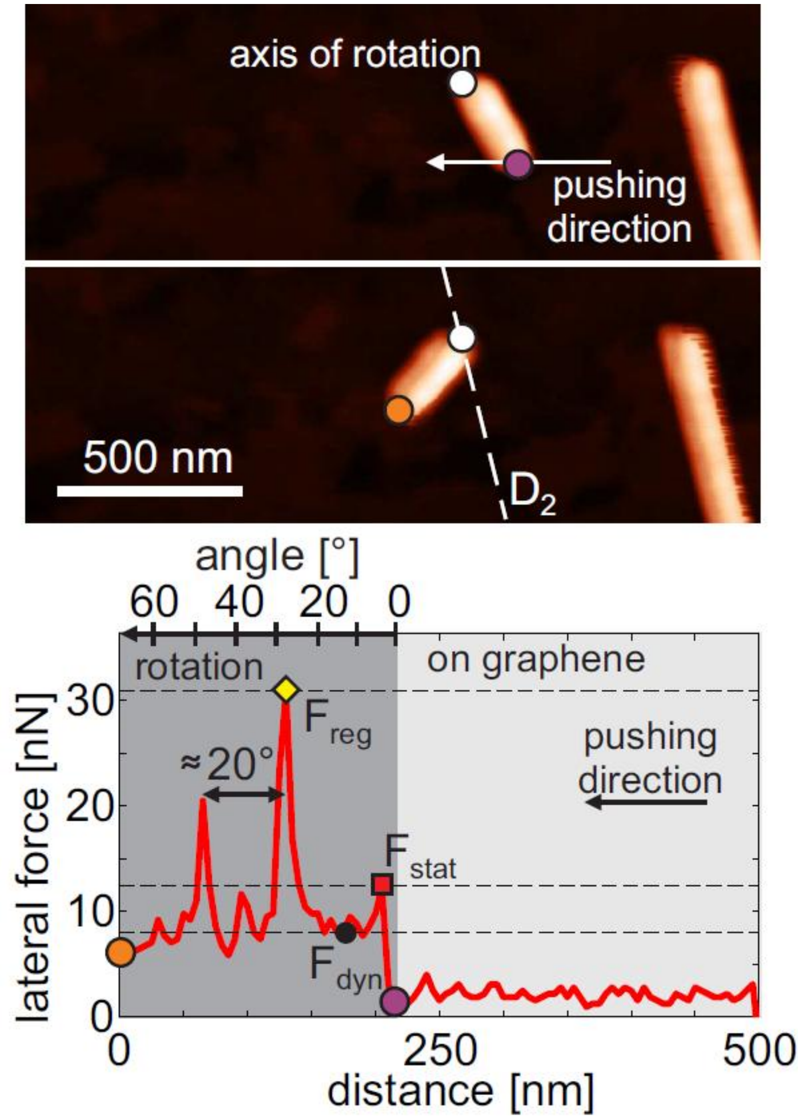




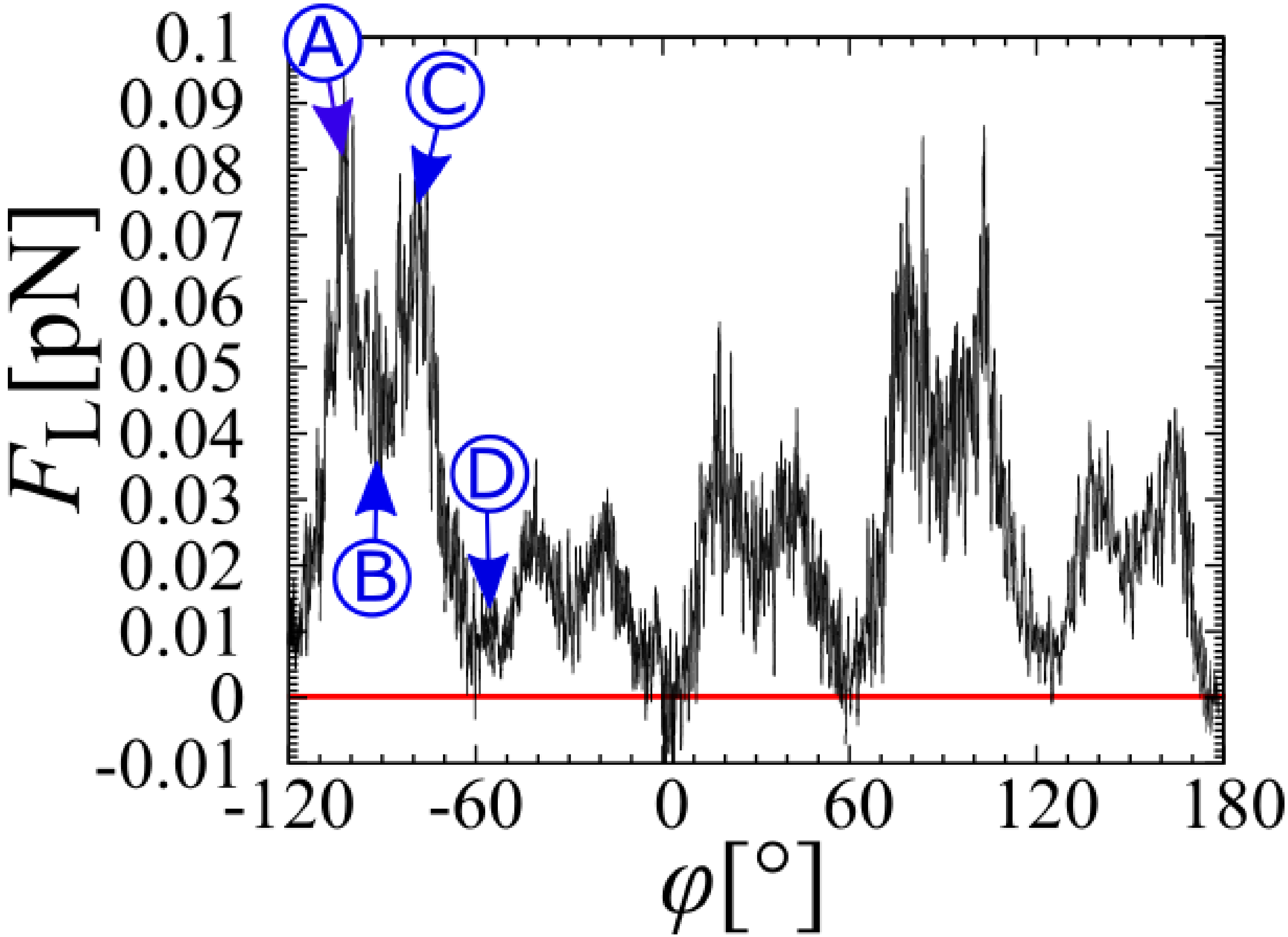
layer moving
as rigid body
rigid graphene
layer
mobile
molecules
(a) top view
y
x
z
(b) side view
z
y
x
(c) bottom view
y
x
z



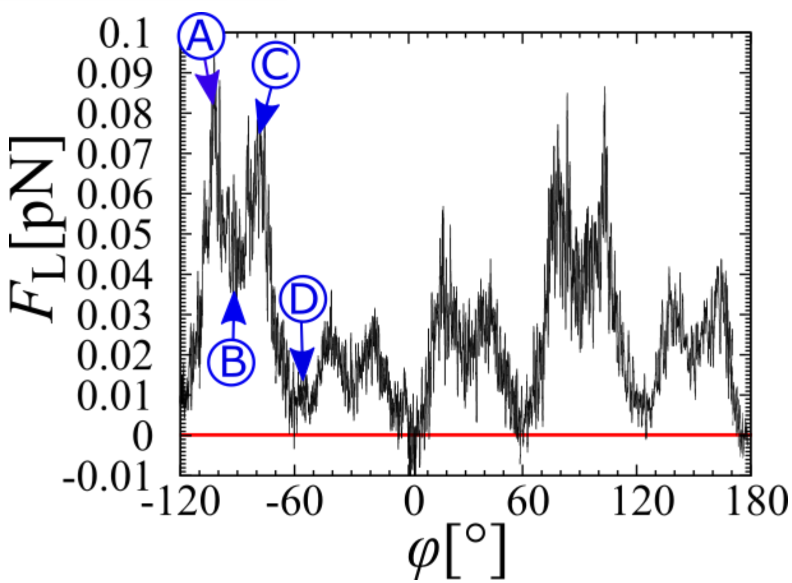
Rotation over the “tracks”

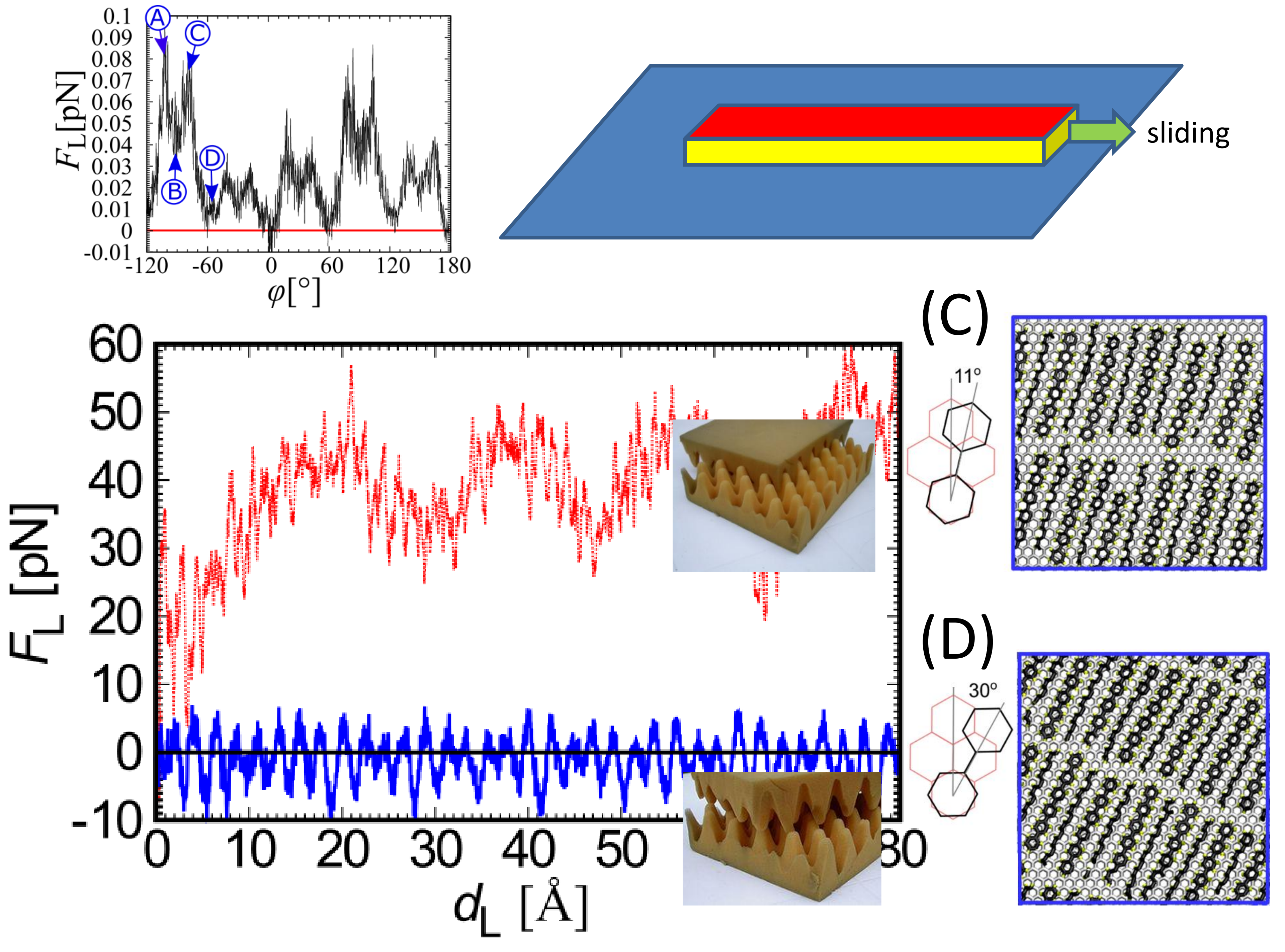


Rotation over the "tracks"

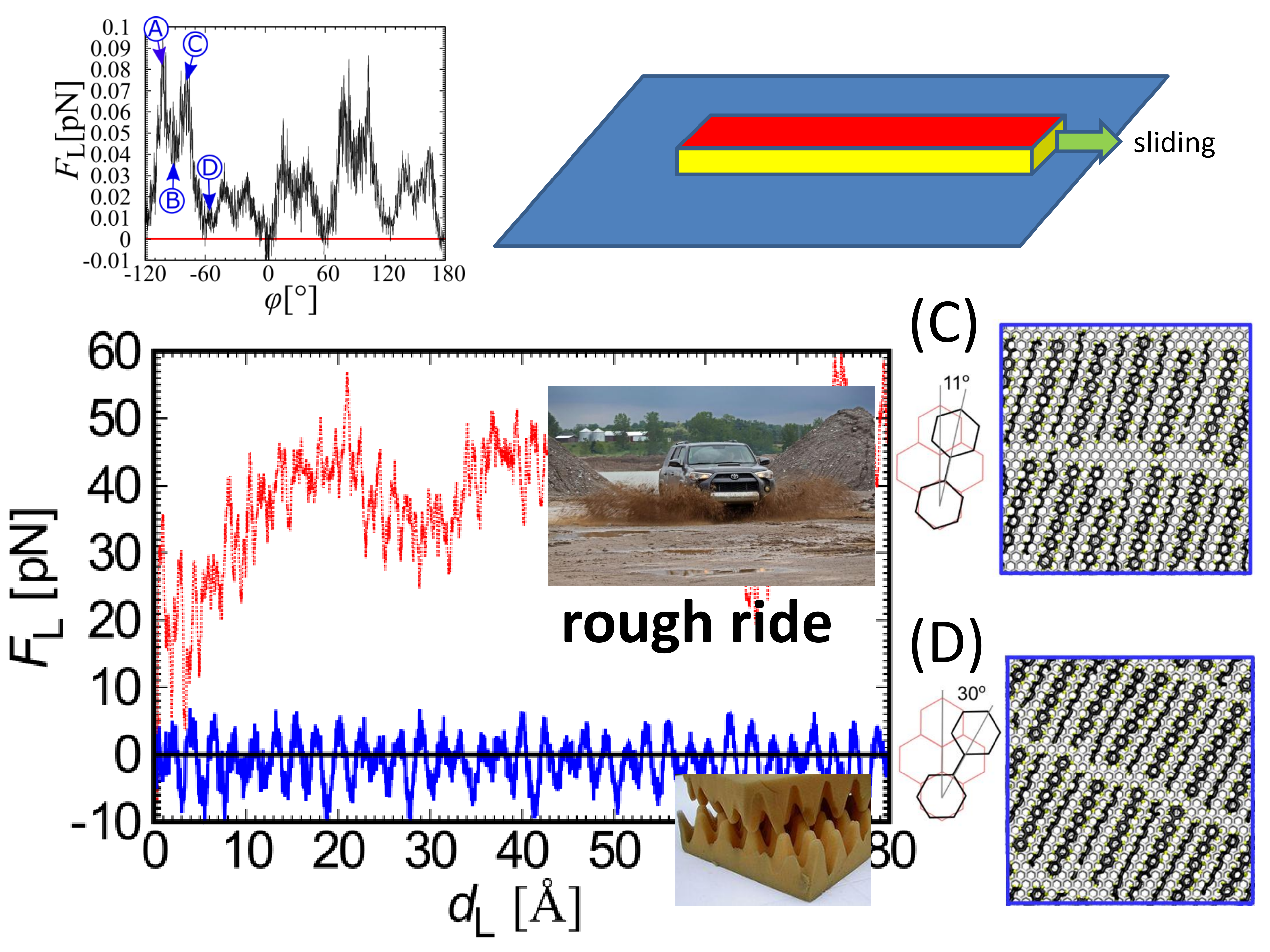



sliding


0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
-0.01
F_L[pN]
A
B
C
D
-120
-60
0
60
120
180
φ[°]



A
B
C
D
F_L [pN]
φ[°]
-120 -60 0 60 120 180
0.1 0.09 0.08 0.07 0.06 0.05 0.04 0.03 0.02 0.01 0 -0.01
sliding
(C)
11°
(D)
30°
F_L [pN]
60 50 40 30 20 10 0 -10
d_L [Å]
0 10 20 30 40 50 80

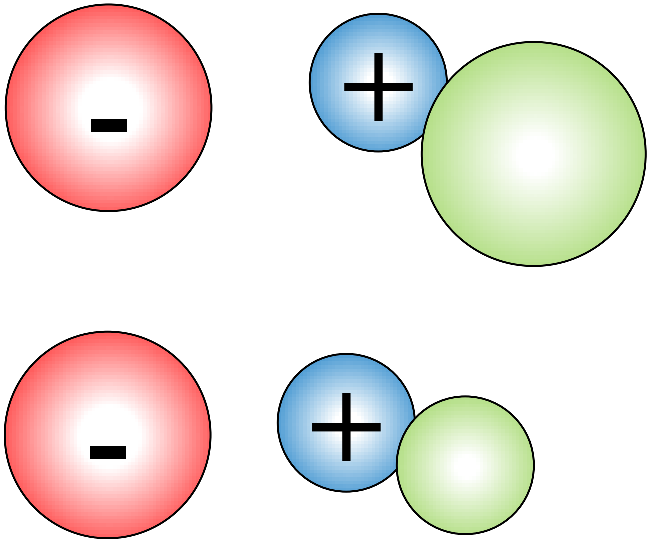


0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
-0.01
A
B
C
D
F_L [pN]
-120
-60
0
60
120
180
φ[°]
sliding
60
50
40
30
20
10
0
-10
F_L [pN]
rough ride
0
10
20
30
40
50
80
d_L [Å]
(C)
11°
(D)
30°

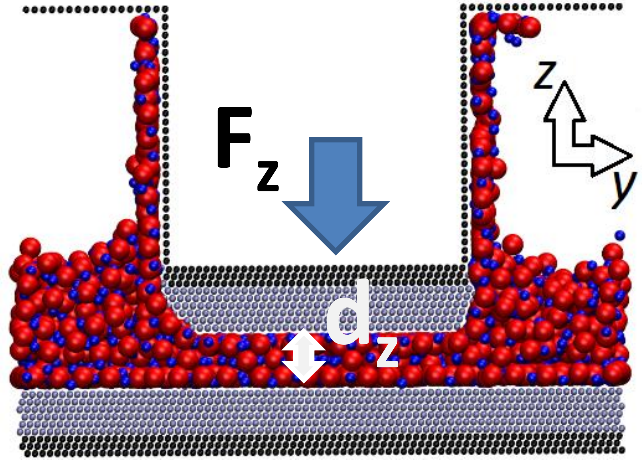
Ionic liquids

Questions:

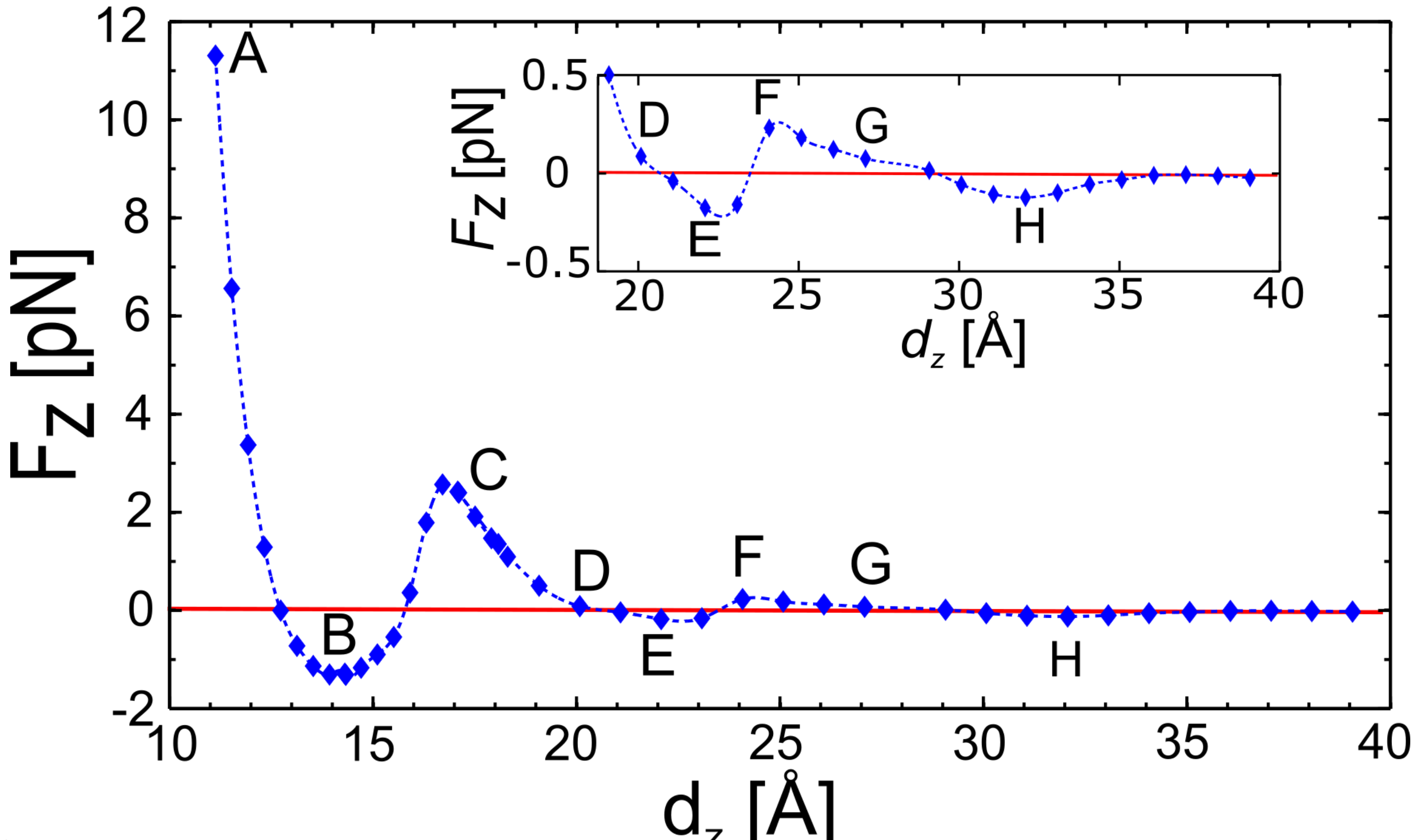
How does molecular structure of IL influences its properties?



What are generic features of IL's response to mechanical excitation?

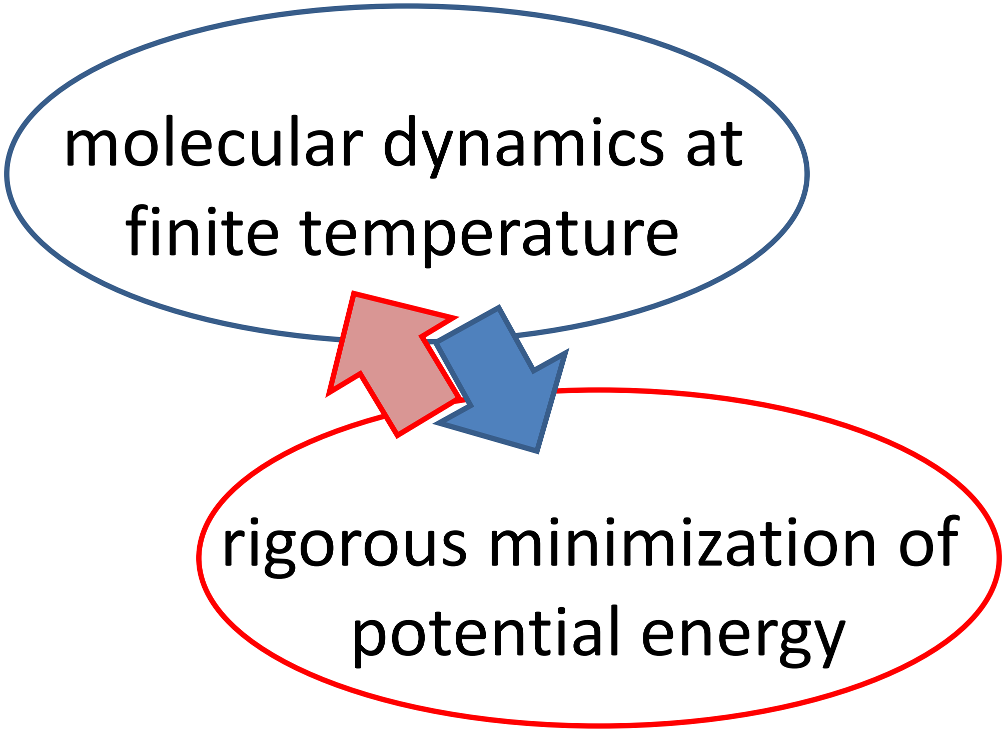


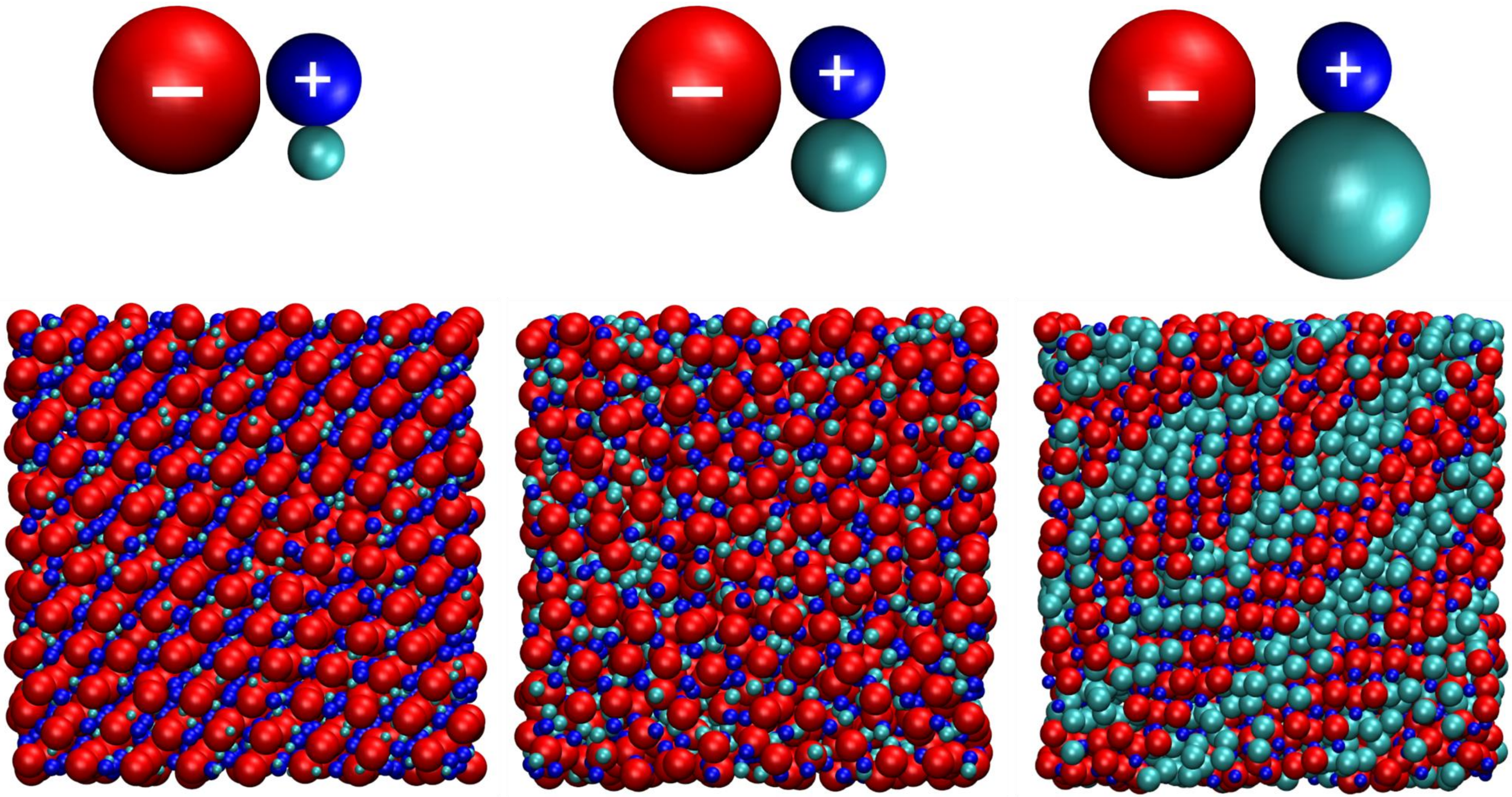
F_z
d_z
z
y



A
B
C
D
E
F
G
H
F_Z [pN]
d_z [Å]

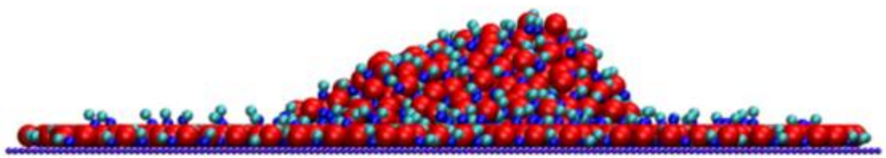
Closed gap between thermal motion & diffusion limited dynamics

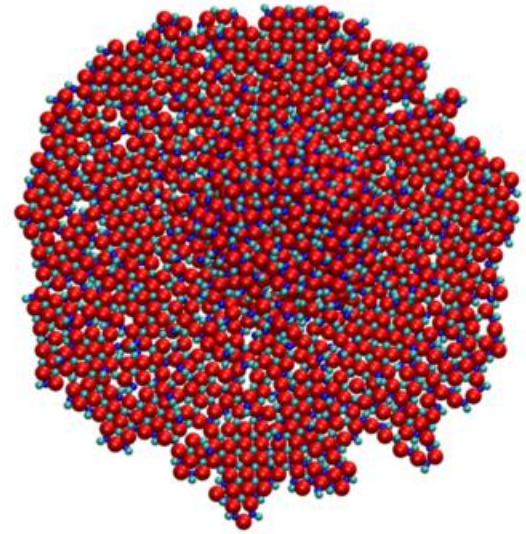




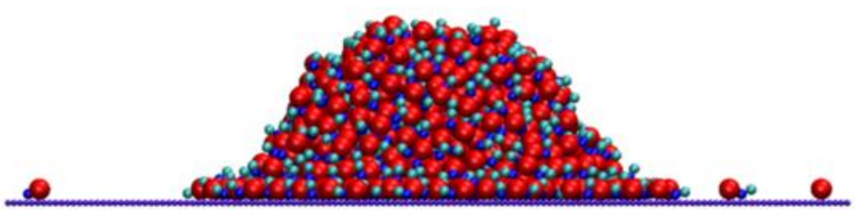
simple cubic　　liquid　　layers

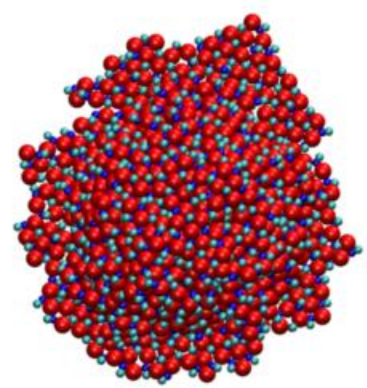
$\varepsilon_{II} = 1.1$, $\varepsilon_{IP} = 5.3$ [kcal/mol]



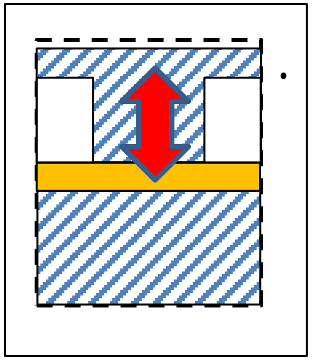


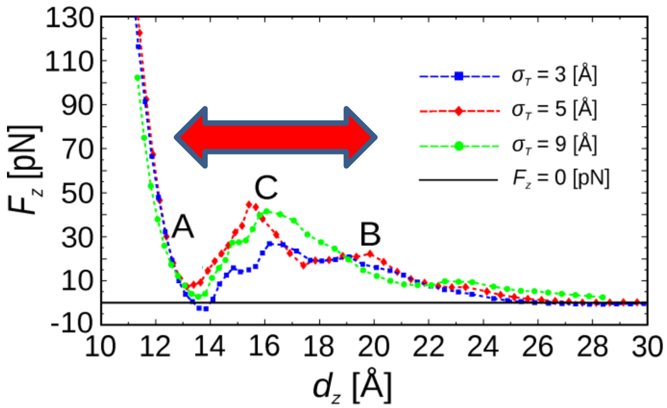
$\varepsilon_{II} = \varepsilon_{IP} = 1.1$ [kcal/mol]

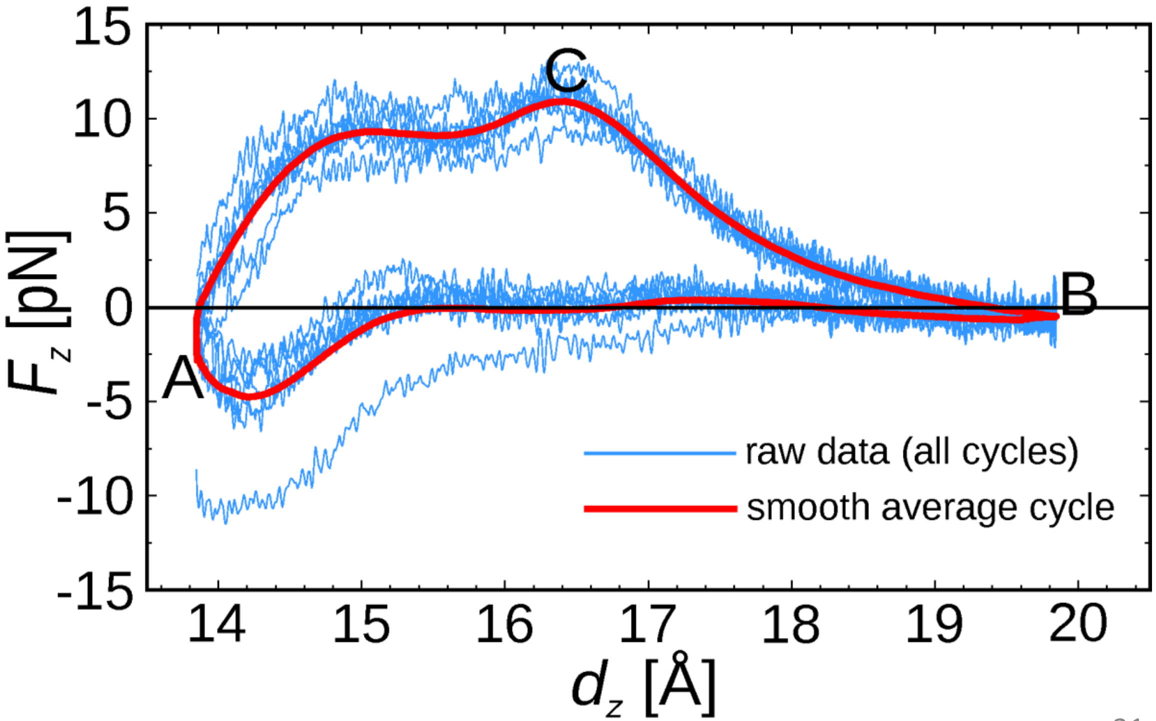


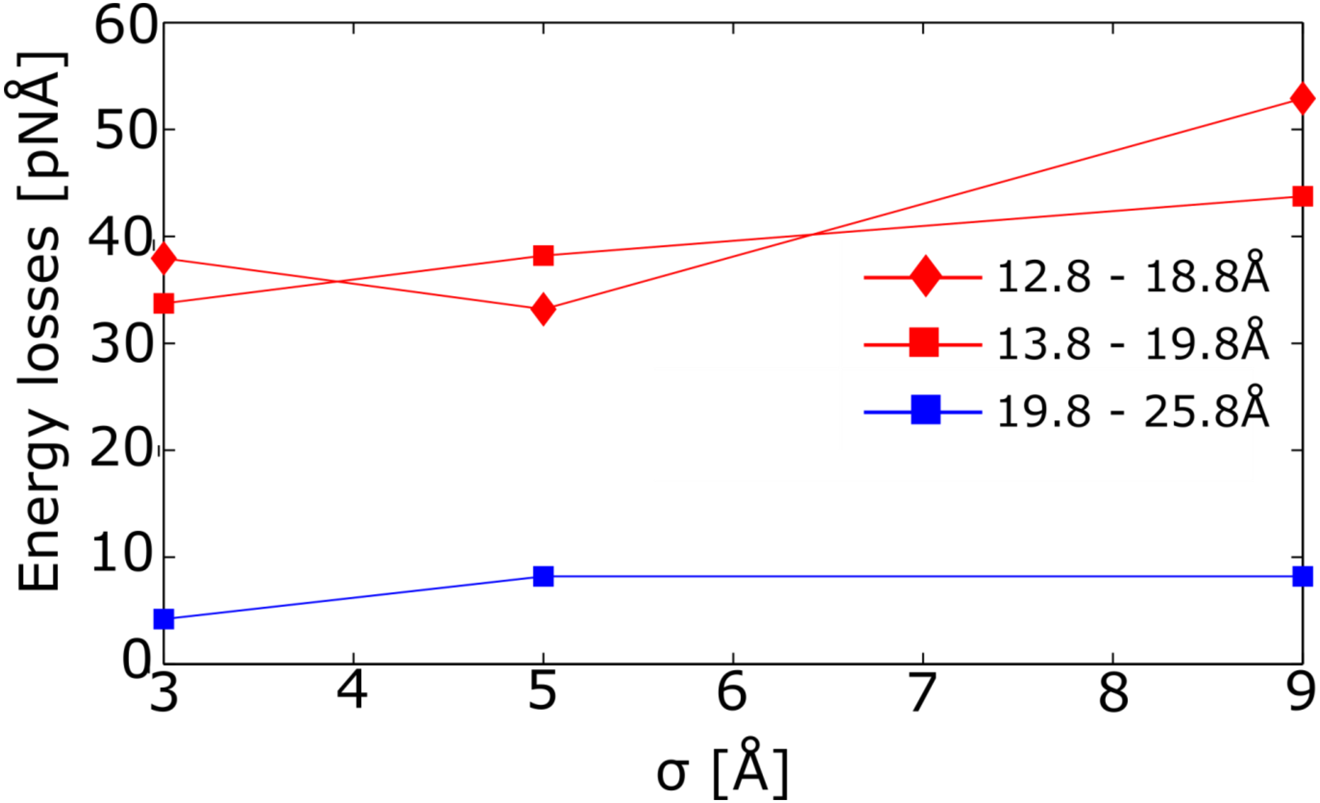


Normal force vs. plate distance









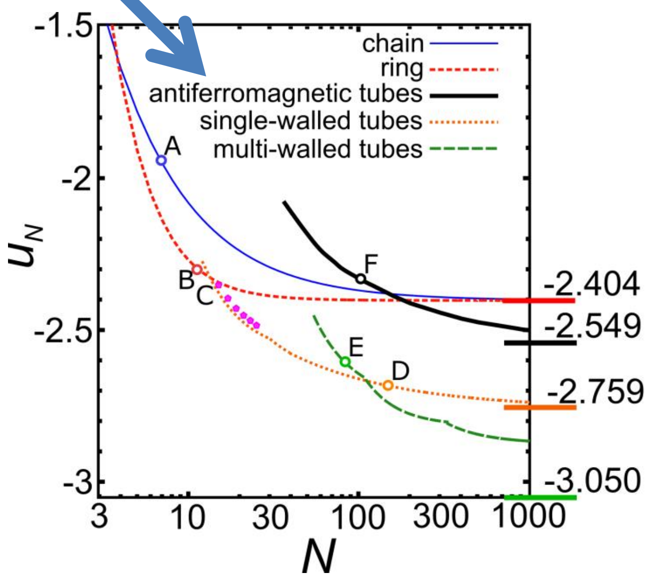
Wall slip as key source of low losses.

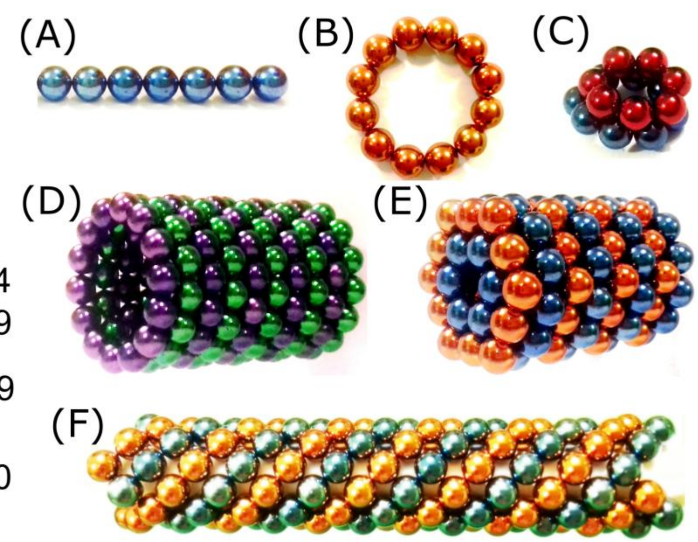
We continue with long range interactions but we change to magnetic interactions.

A brief history of magnetism

Minimal energy structures?

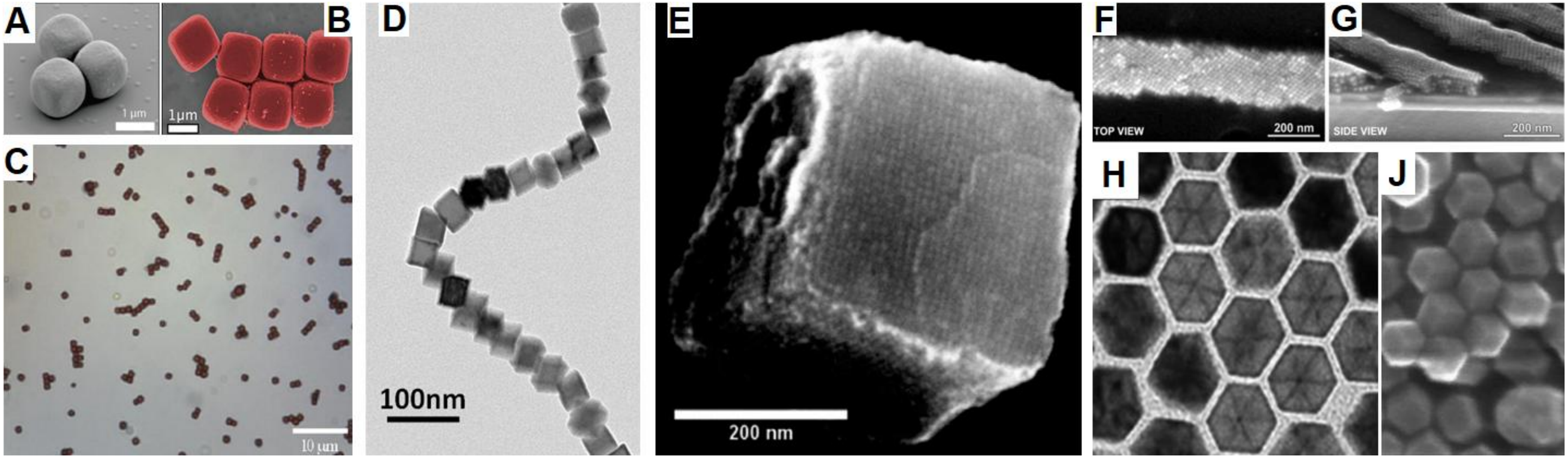
I. S. Jacobs and C. P. Bean, Phys. Rev. 100, 1060 (1955).
P. G. de Gennes and P. A. Pincus, Phys. Kondens. Mater. 11, 189 (1970).

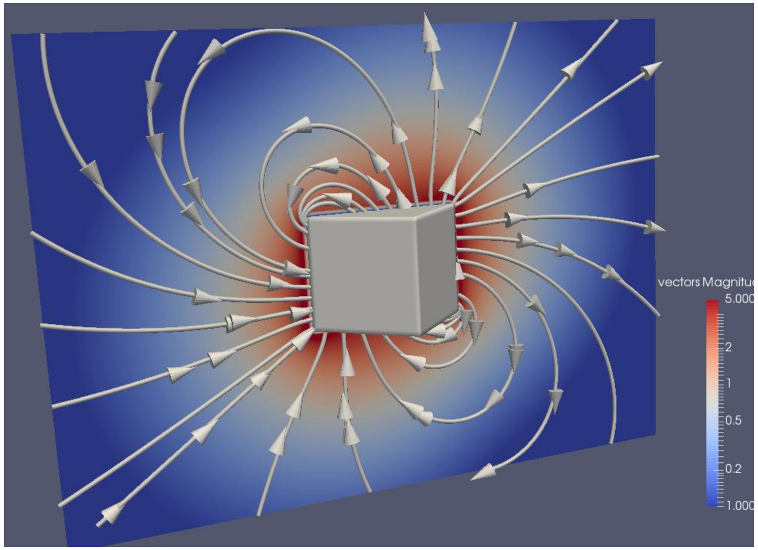




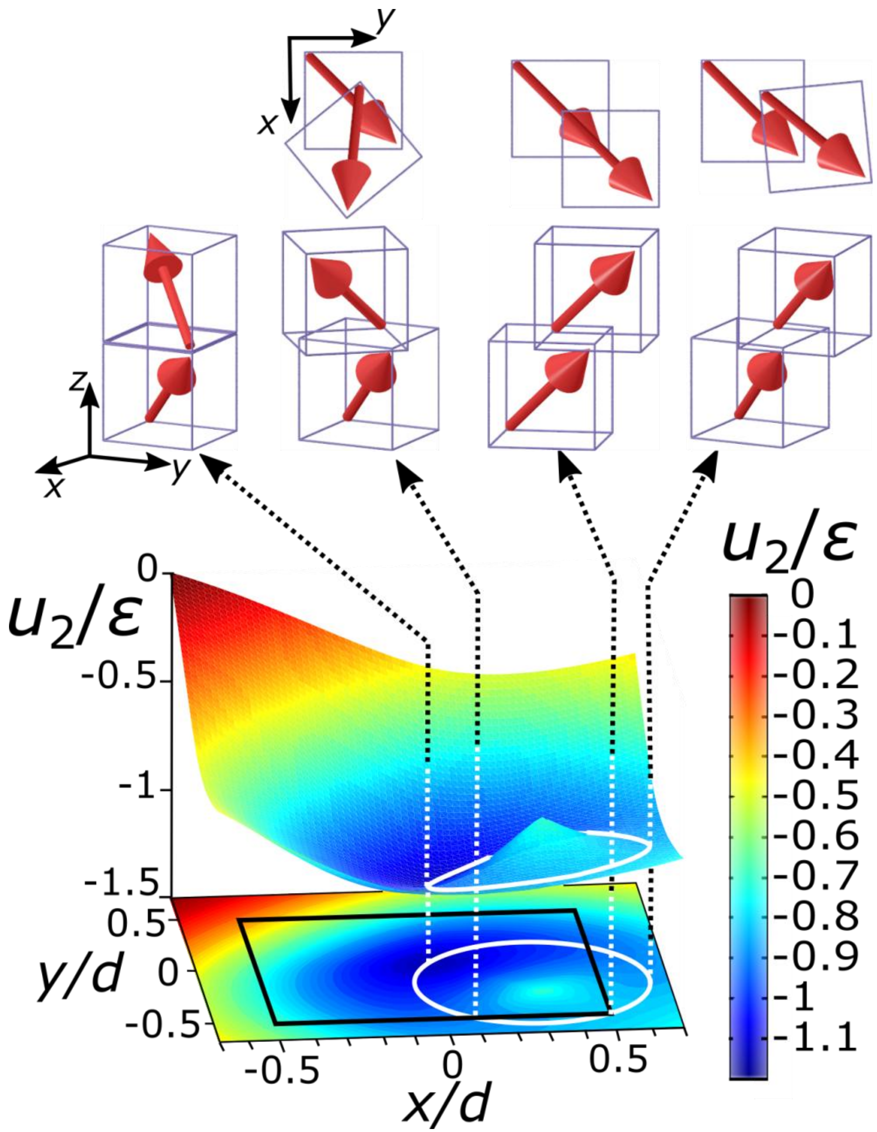
IS, M. Dasic, J. Otalora , C. Garcia, A Platform for Nanomagnetism – Assembled Ferromagnetic and Antiferromagnetic Dipolar Tubes, Nanoscale 11, 2521 (2019).

from magnetic spheres to magnetic cubes…



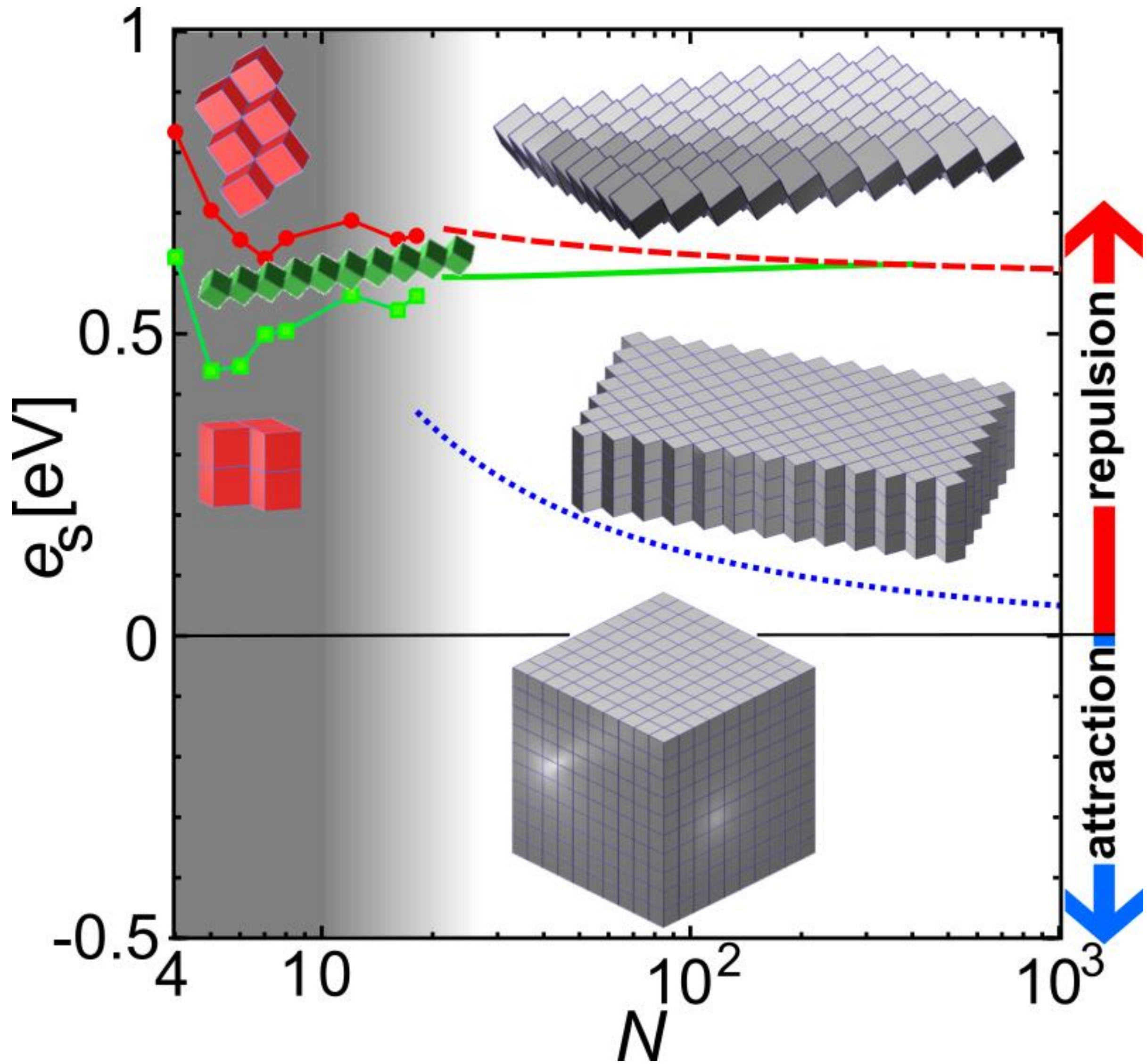


What about just two cubes?

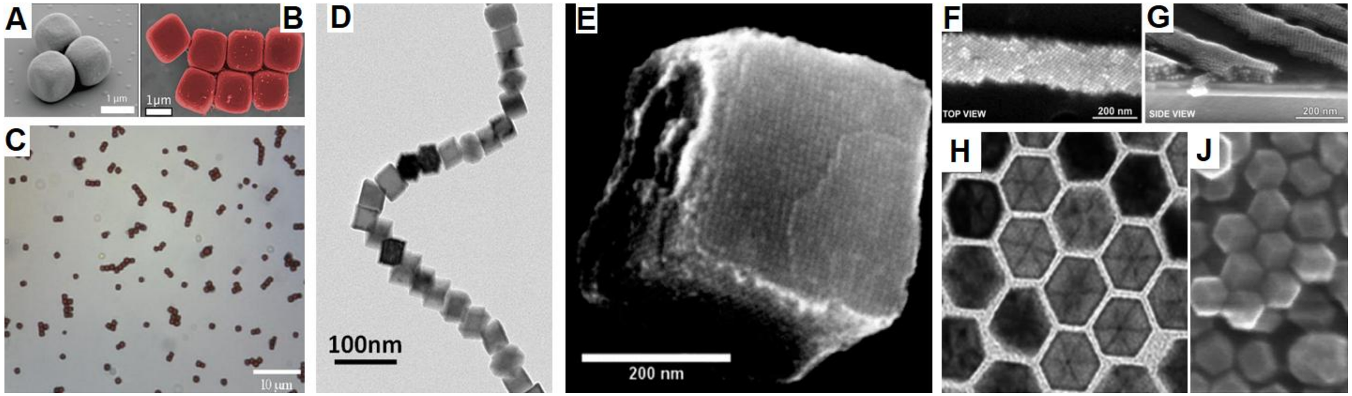


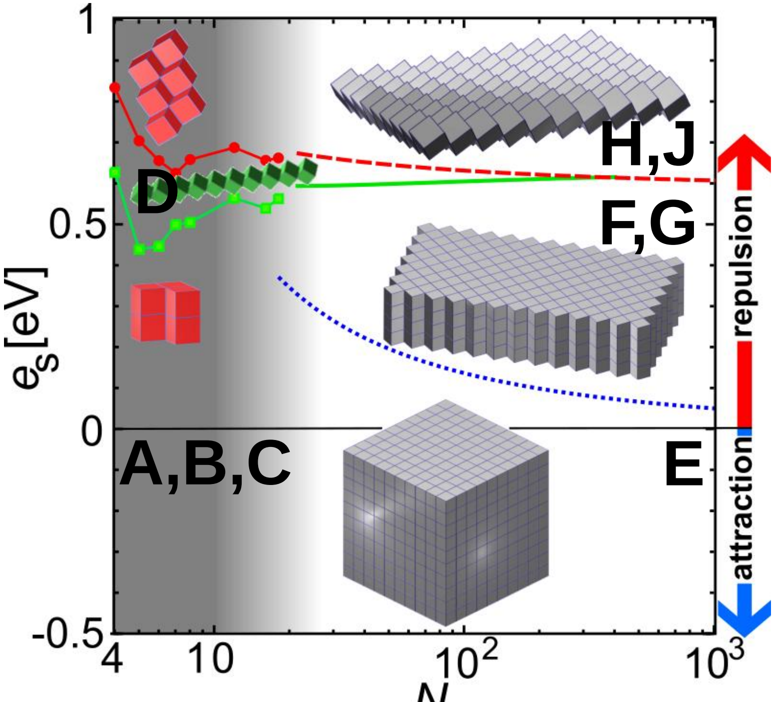
L. Balcells, **IS**, Z. Konstantinovic, A. Alagh, V. Fuentes, L. Lopez-Mir, J. Oro, N. Mestres, C. Garcia, A. Pomar, B. Martínez, Spontaneous In-flight Assembly of Magnetic Nanoparticles into Macroscopic Chains, Nanoscale 11, 14194-14202 (2019).

and if we add surface interactions…

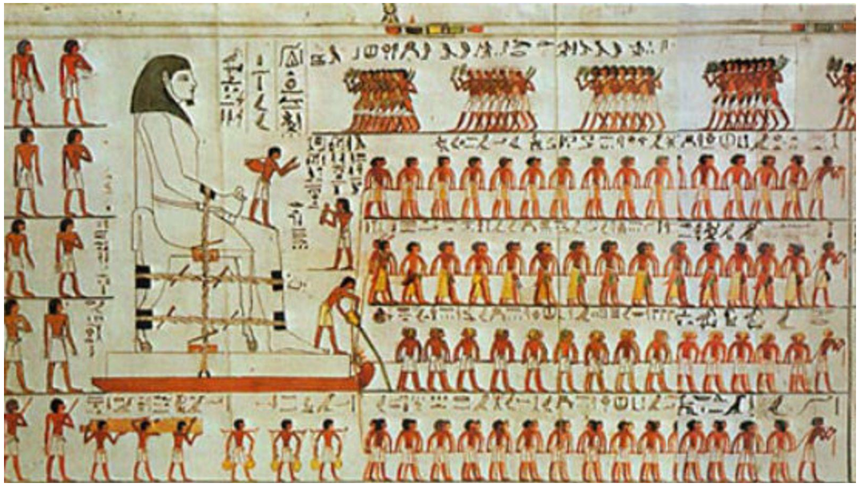


and if we add surface interactions…





and future...



Thank you!