Milan, April 16, 2013

Static and dynamic friction in sliding colloidal monolayers

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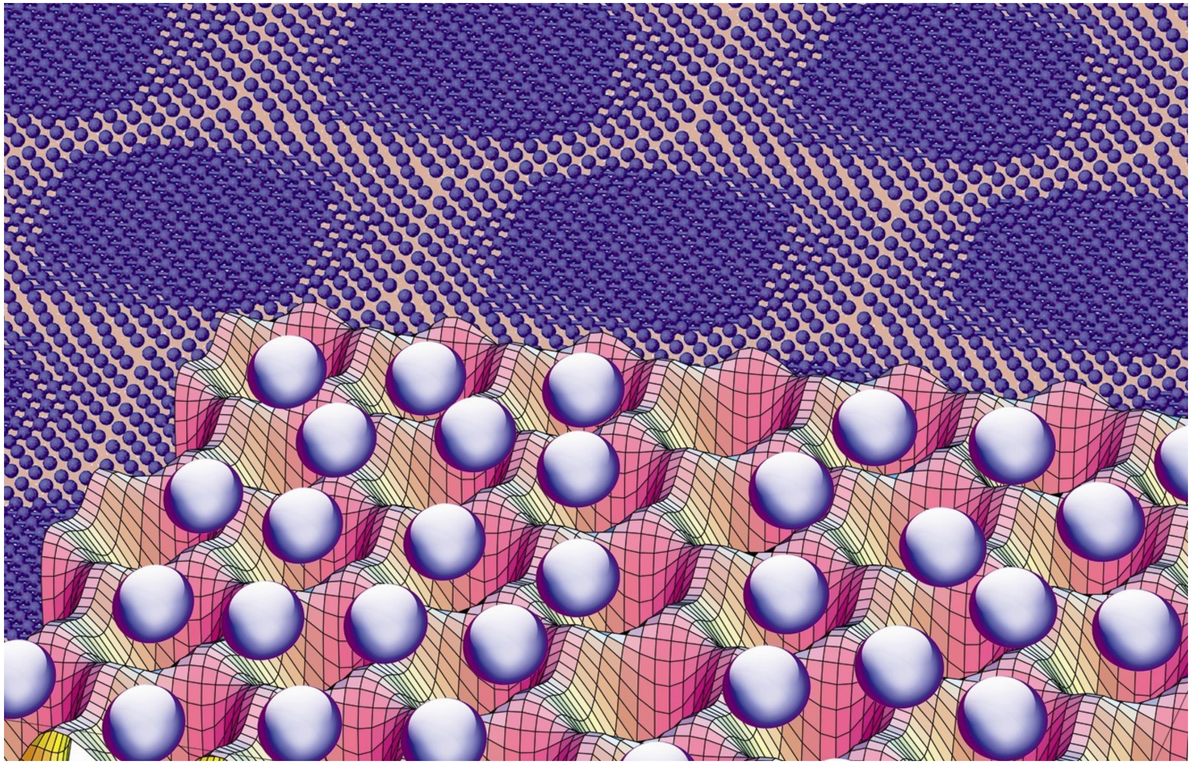
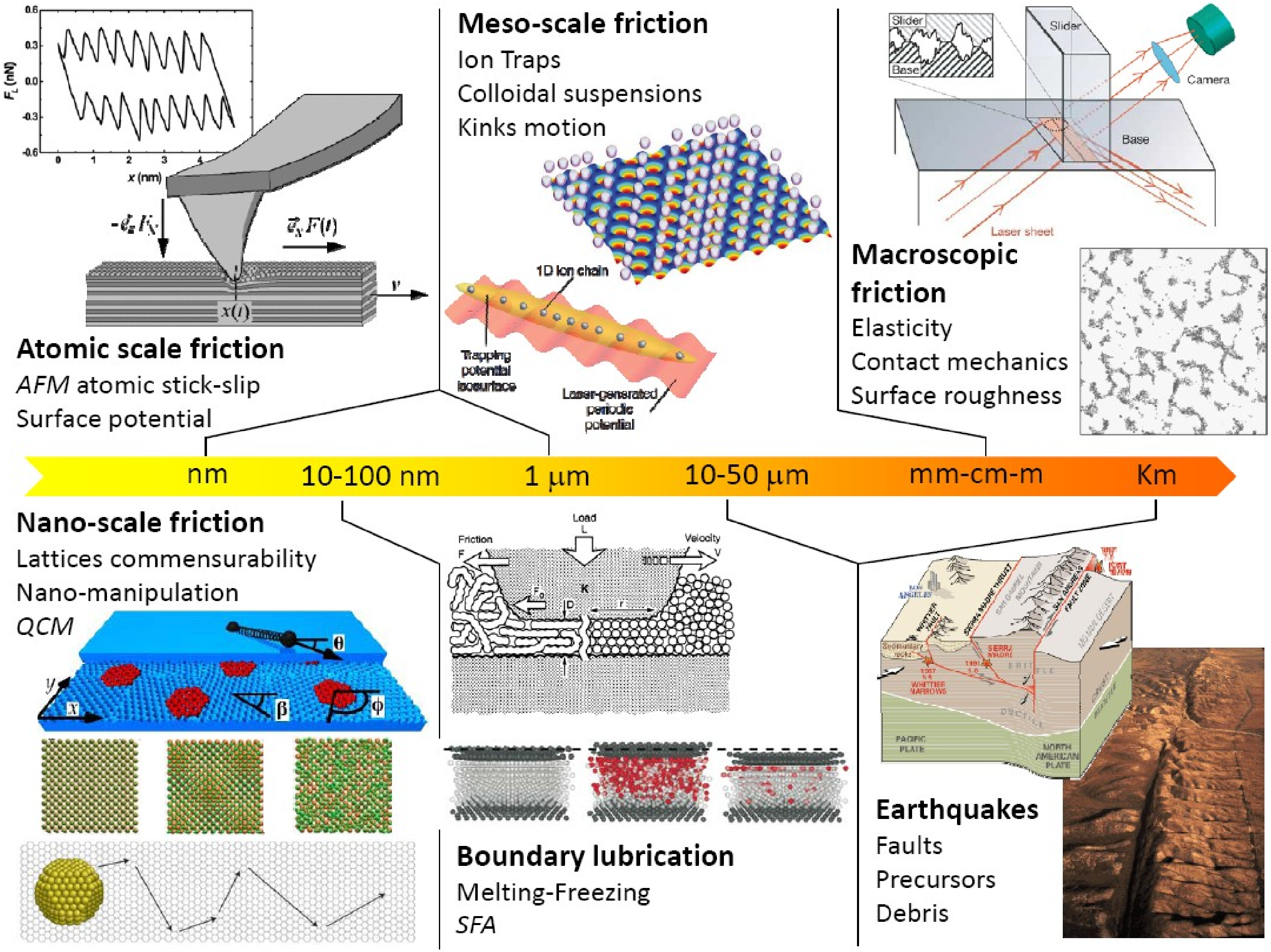


in collaboration with: **A. Vanossi**, **E. Tosatti** (*Trieste*)

Outline

- *(Nano) friction at a glance*
- *Driven colloidal monolayers as a model system for nanotribology*
- *Experimental findings: role of topological solitons*
- *MD modeling of driven colloidal monolayers*
- *Static and dynamic friction*
- *Summary and Outlook*

(Nano-) friction at a glance



- Friction spans all length scales, from micro up to macro
- It involves high-nonlinear out-of-equilibrium processes usually at a buried interface

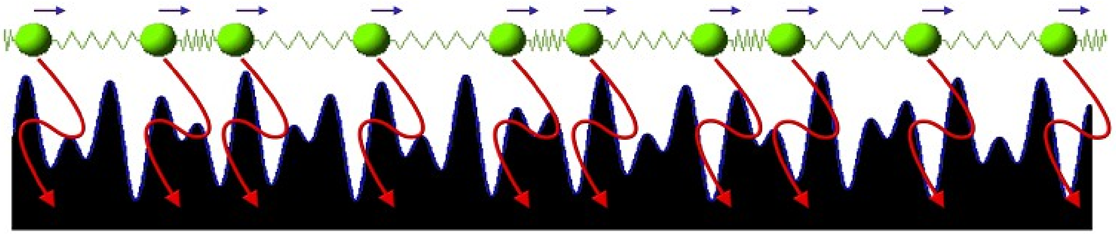
Why studying friction?

- Fundamental understanding of interface mechanisms
- Bridging the gap between micro and macro
- (Nano)Technology, applications and energy/materials saving (~ 6% GNP lost to friction)

Controlling friction is crucial

(Nano-) friction at a glance

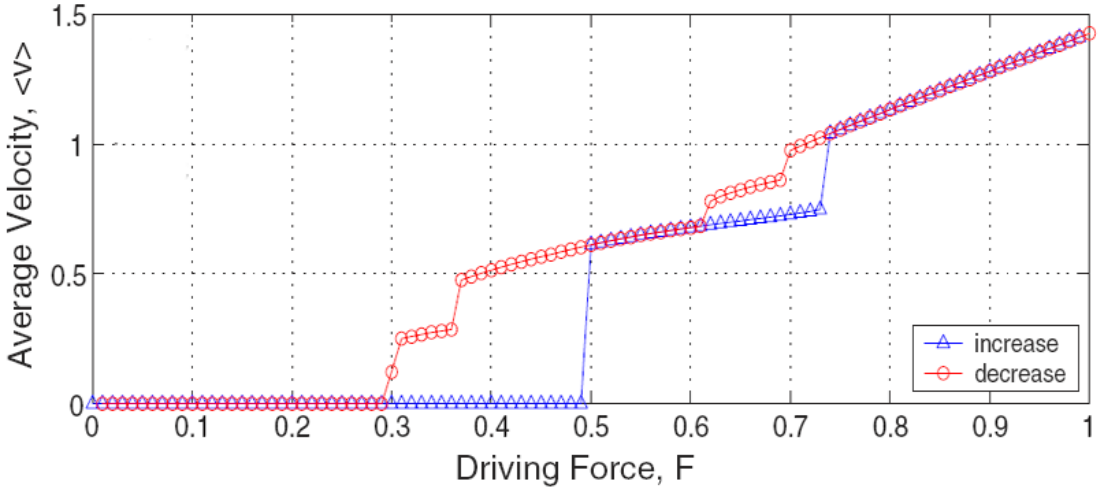
Studying friction usually means describing the *dissipative dynamics of a slider* (e.g., a chain of interacting particles) *moving over a surface* (e.g., a rigid / deformable / periodic / disordered substrate potential) *due to the application of an external force*.



How does the system respond to external driving ?

- What are the features at the basis of:
  - *pinning*
  - *depinning transition*
  - *sliding regimes*
  - *stick-slip and smooth dynamics*
  - *superlubricity*
  - *energy dissipation*
  - *…* ?

- In general, *the mobility is a highly **nonlinear** function of the force*.



Urbakh et al., Nature 430, 525 (2004).
Muser et al., Adv. Chem. Phys. 126, 187 (2003).

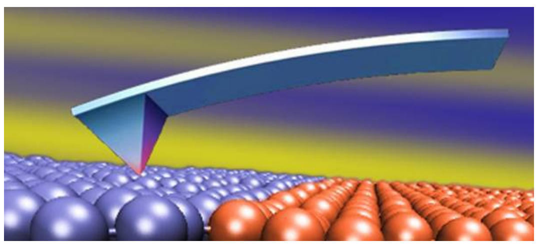
Vanossi and Braun, J. Phys.: Condens. Matter 19, 305017 (2007).

(Nano-) friction at a glance

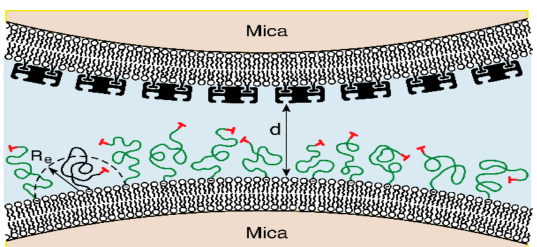
How to study all that?

Fundamental understanding begins at the smaller scales, where the basic processes are involved and *experiments at well-characterized interfaces* are now possible

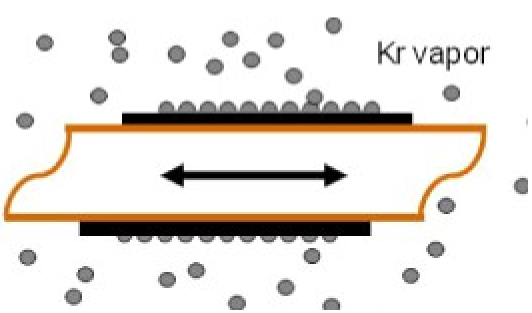
Experimentally



AFM/FFM



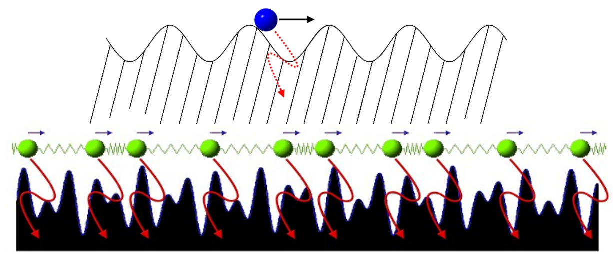
SFA



QCM

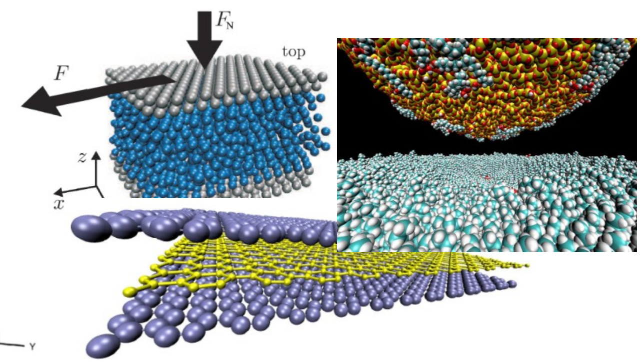
Carpick and Salmeron, Chem. Rev. 97, 1163 (1997)

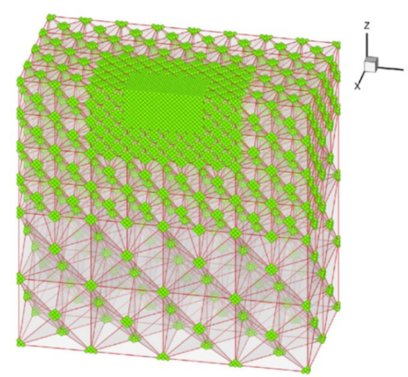
Theoretically



Minimalistic

MD





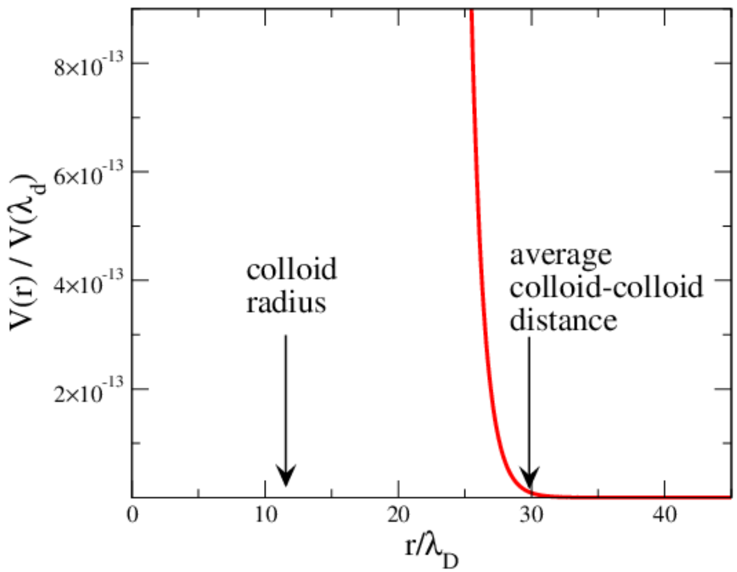
Multiscale

Robbins and Muser, in Modern Tribology Handbook (2001)
Vanossi, Manini, Urbakh, Zapperi, Tosatti, Rev. Mod. Phys, 2013

Friction in driven colloidal monolayers

- **Replace atoms with micron-sized colloidal particles**
- **Create substrate potentials with optical light fields**

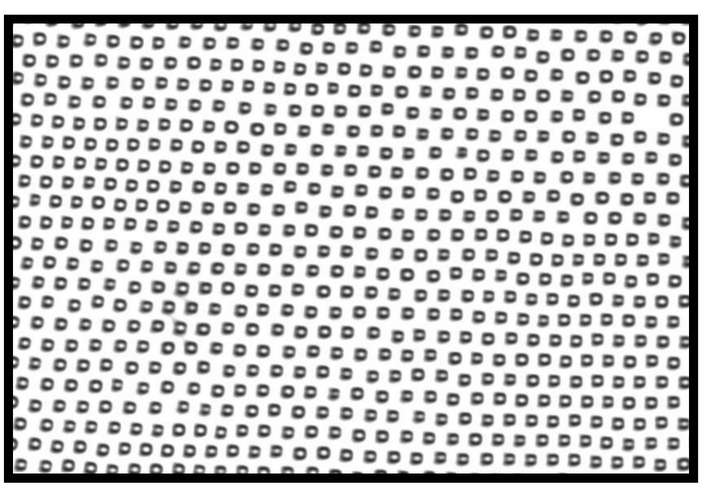
Specifically: highly charged polystyrene spheres (R=1.95 μm) suspended in water



Repulsive screened electrostatic-pair potential

$$V(r) = (Q/r)\exp(-r/\lambda_D)$$

with the Debye screening length λ_D (= 0.16 μm << R) tuned by the ion concentration of the suspension



Formation of a 2D hexagonal crystal under confinement

Baumgartl, Brunner, Bechinger, PRL 93, 168301 (2004); Baumgartl, Zvyagolskaya, Bechinger, PRL 99, 205503 (2007).

Driven colloidal monolayers

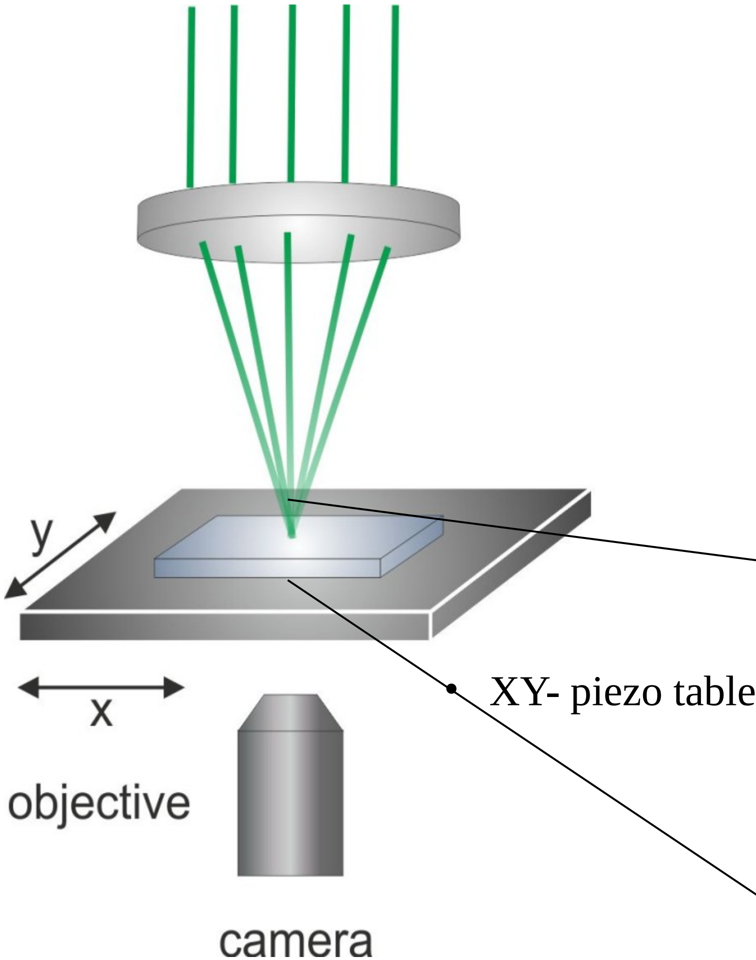
Translation of sample cell ⇨ *lateral force*

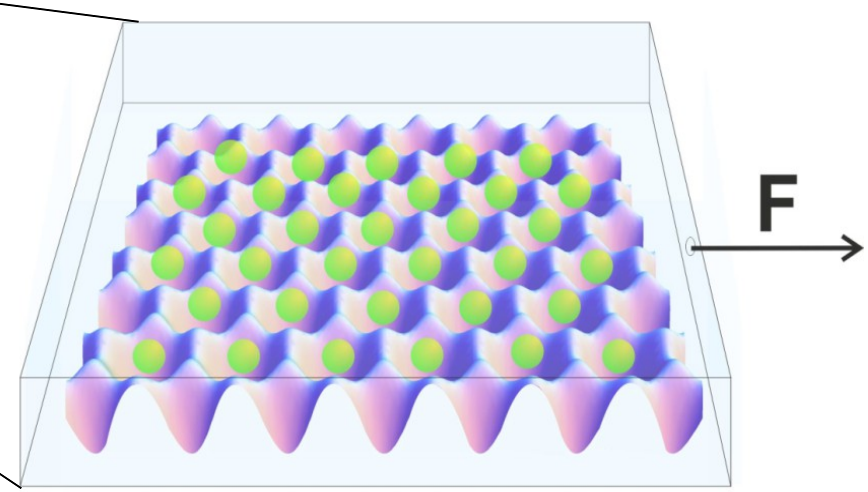
$$\mathbf{F} = \gamma_{\mathrm{eff}}\, v_{\mathrm{cell}}$$

Free sphere: $\gamma_{\mathrm{eff}} = 6\,\pi\,\eta\,r$

- *Here: wall + surrounding particles*

$$\gamma_{\mathrm{eff}} = \frac{k_B T}{D_{\mathrm{eff}}}$$





Particle positions are observed in real space (and time) with high precision (20 nm)

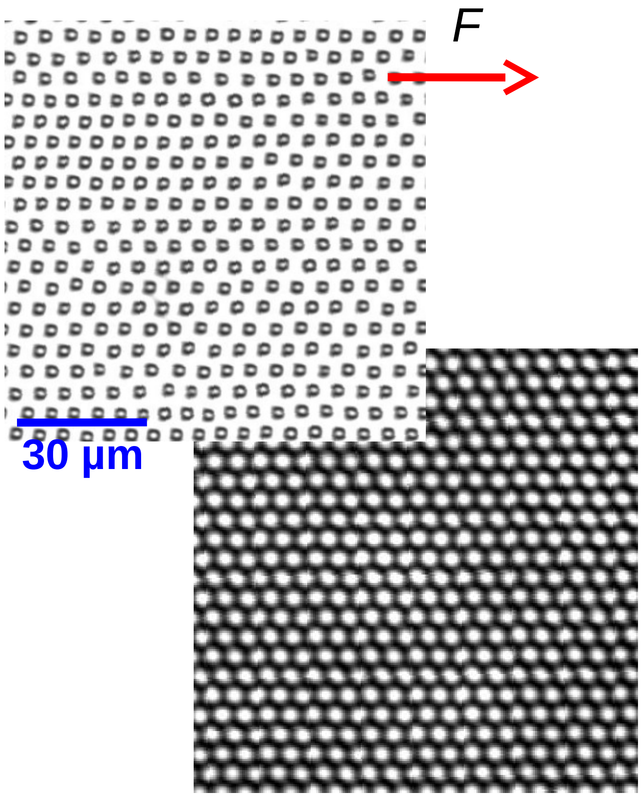
adjustable strength, geometry and length scale of substrate potential !!

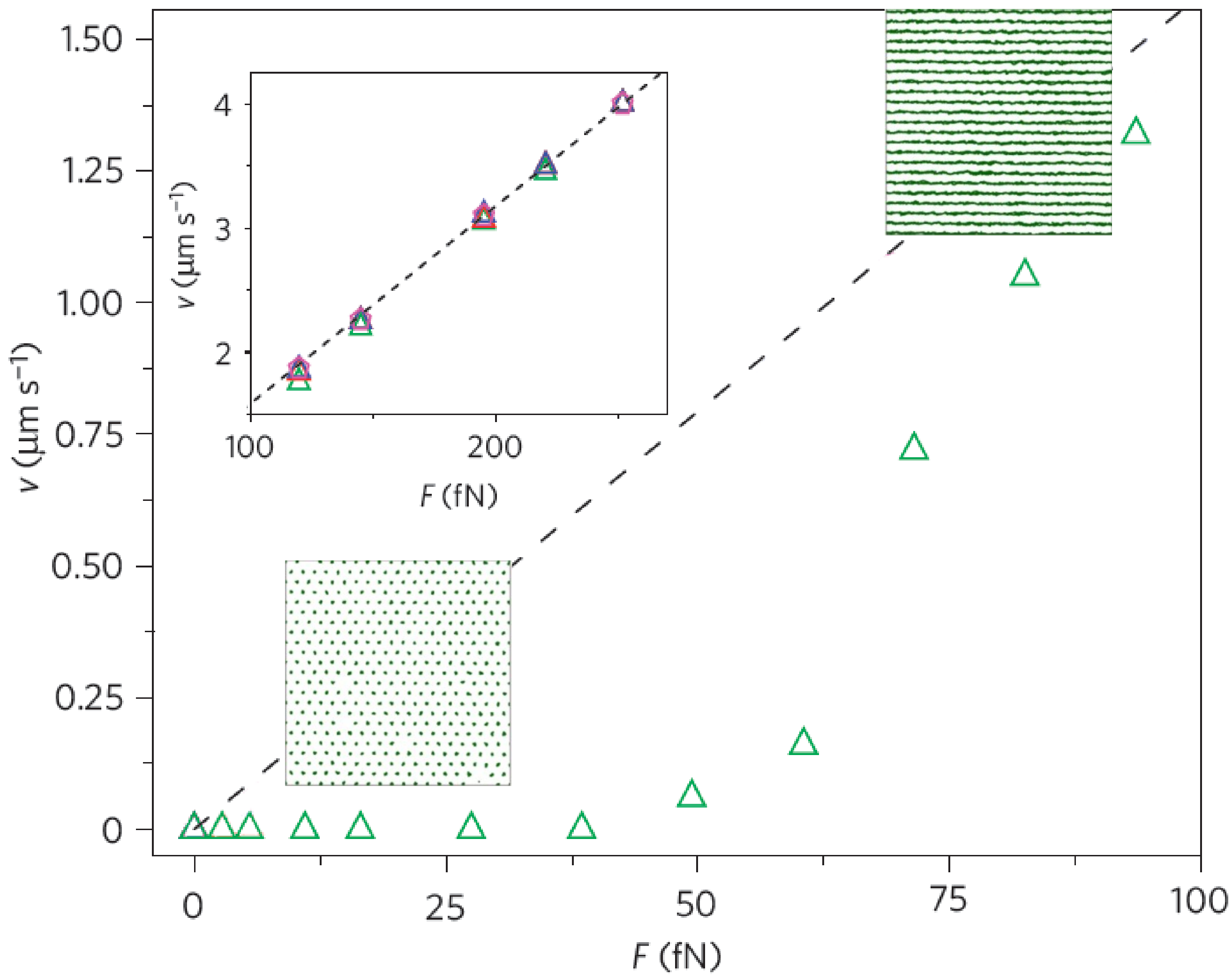
Bohlein, Mikhael and Bechinger, Nat. Mater. 11, 126 (2012)

Experimental findings

Friction of a colloidal crystal on a periodic substrate

commensurate case $a_{coll} = a_{sub}$ (= 5.7 μm)

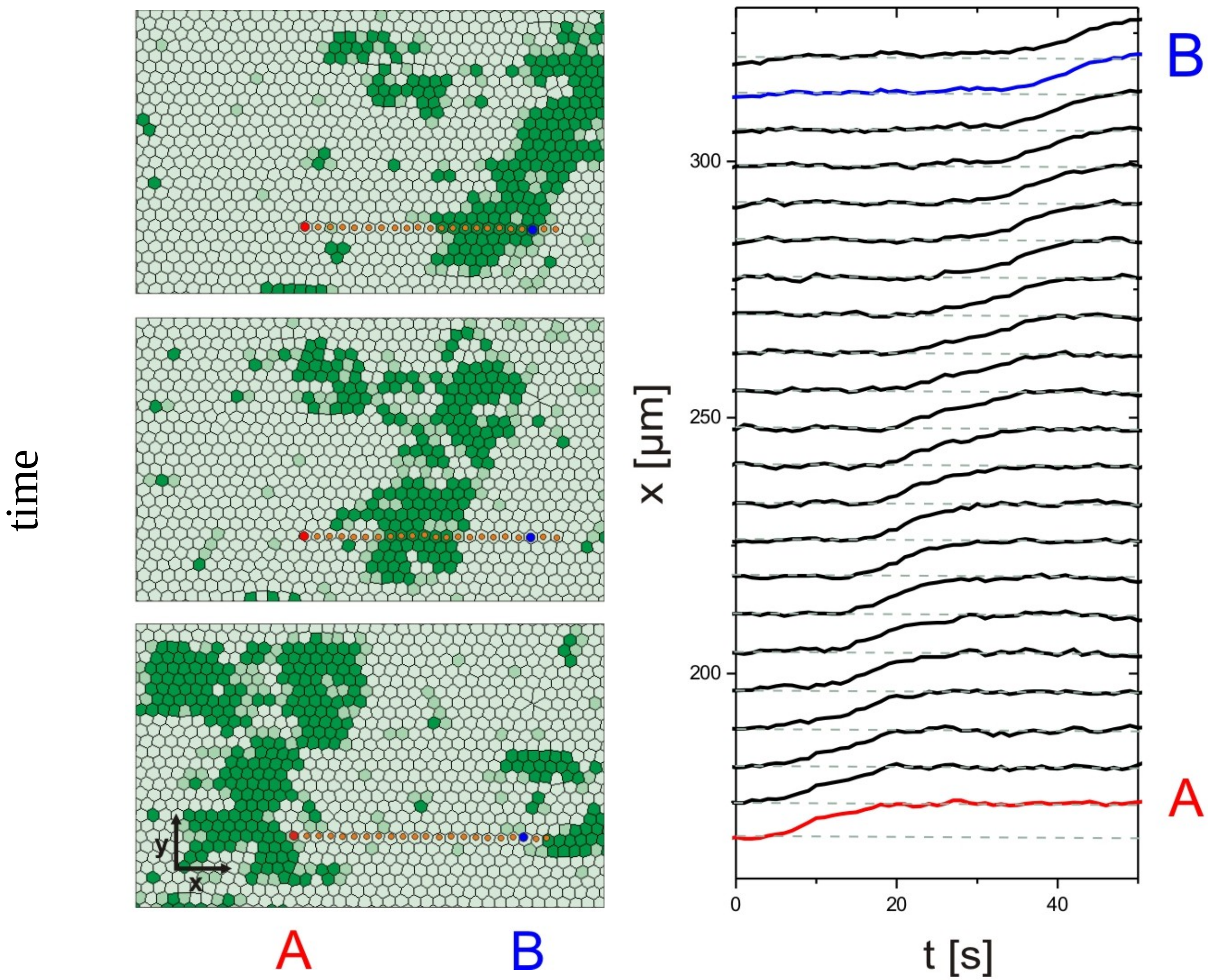




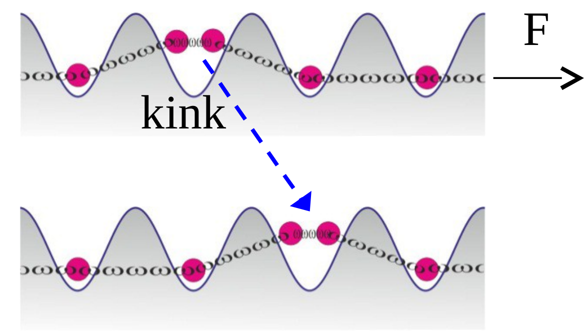
Bohlein, Mikhael and Bechinger, Nat. Mater. 11, 126 (2012)

Experimental findings

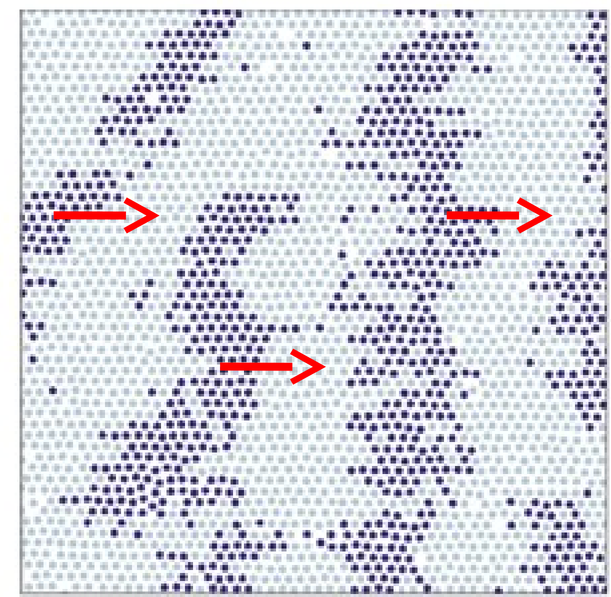
just above the depinning transition...



fast particles coincide with compressed areas



mass transport occurs via the translation of kinks



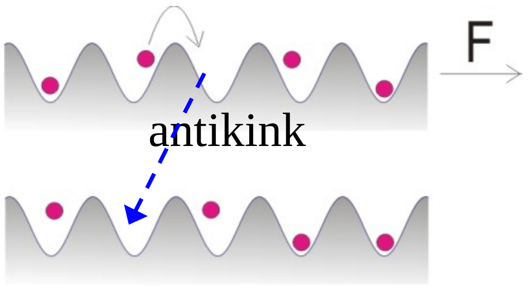
...at higher driving

Why kinks at a commensurate interface ???

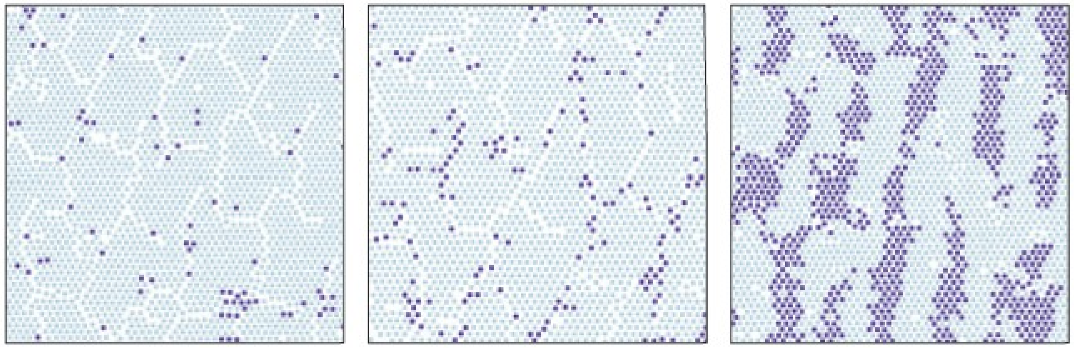
Experimental findings

Friction of a colloidal crystal on a periodic substrate

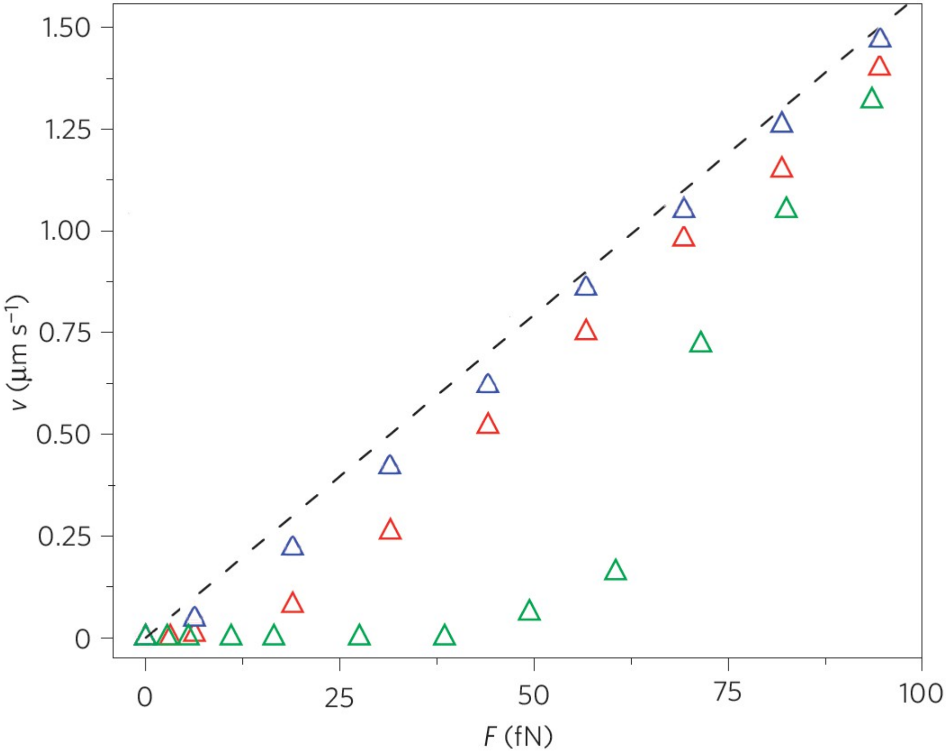
incommensurate case $a_{coll} > a_{sub}$



Increasing driving force



Fast particles coincide with expanded areas



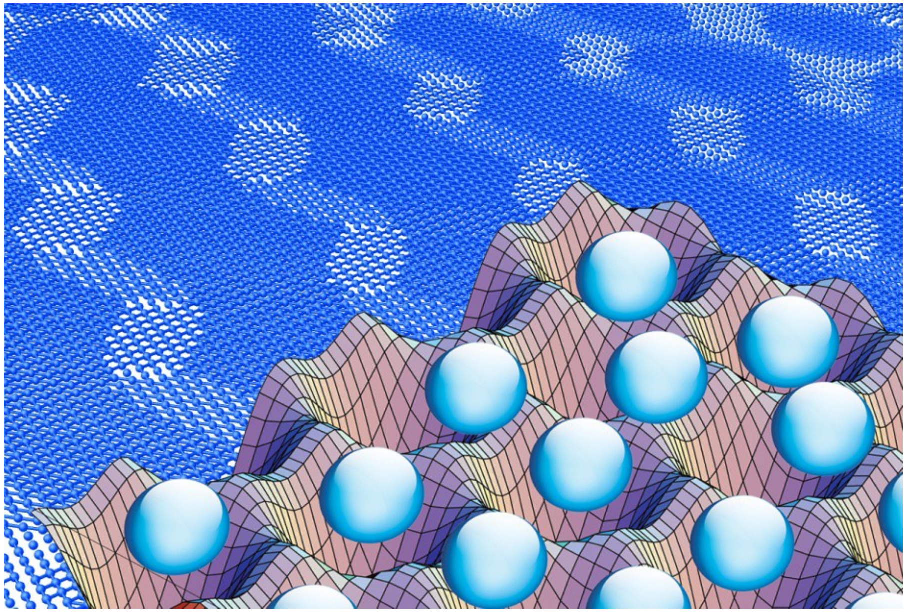
Static friction is largely reduced due to preformed antikinks

$a_{coll} = 5.7\,\mu m$

$a_{sub} = 5.7\,\mu m$ $a_{sub} = 5.2\,\mu m$ $a_{sub} = 4.8\,\mu m$

toward **superlubricity**

MD modeling



- modelled as charged point particles undergoing overdamped 2D dynamics under an external force applied to each colloid

- $V(r_{ij}) = Q/r_{ij}\exp(-r_{ij}/\lambda_D)$
  screened Coulomb repulsion with λD substantially smaller than the mean particle distance

- $F = \eta\, v_d$ (fluid effective viscosity and velocity)

- $-\eta\, v_i$ (Stokes viscous force)

- colloids are immersed in a Gaussian-shaped overall confining potential

$$G(|\mathbf{r}|) = -A_c \exp(-r^2/\sigma^2)$$ (laser spot)

and in a triangular-lattice periodic potential

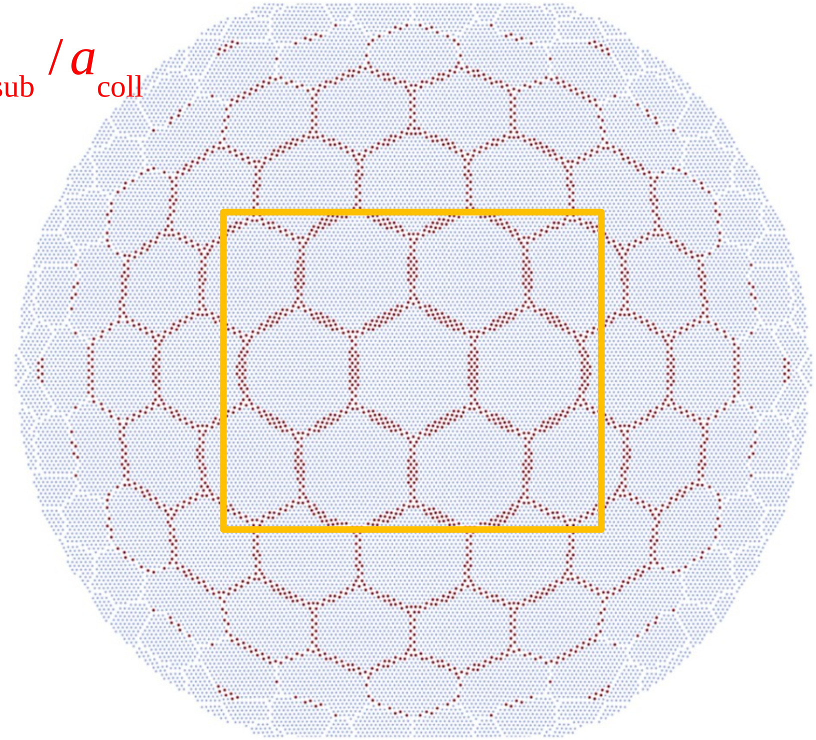
$$W(\vec{r}) = -\frac{2}{9}U_0\left[\frac{3}{2} + 2\cos\frac{2\pi r_x}{a_{\mathrm{sub}}}\cos\frac{2\pi r_y}{\sqrt{3}a_{\mathrm{sub}}} + \cos\frac{4\pi r_y}{\sqrt{3}a_{\mathrm{sub}}}\right]$$ (substrate corrugation)

Vanossi, Manini, Tosatti, PNAS 109, 16429 (2012).

MD modeling

typical simulation size $N \simeq 30{,}000$

- $U_0 = 0$, 2D triangular colloidal lattice island at rest (confining and repulsion energy balance)
- balance setting so that the average $a_{coll} = 1$
- by changing $a_{sub} = 1$, variety of mismatched ratios $\rho = a_{sub} / a_{coll}$
  - 3 representative cases:
    - underdense, $\rho = 0.95$ (AI)
    - nearly commensurate, $\rho \simeq 1.0$ (CO)
    - overdense, $\rho = 1.05$ (SI)



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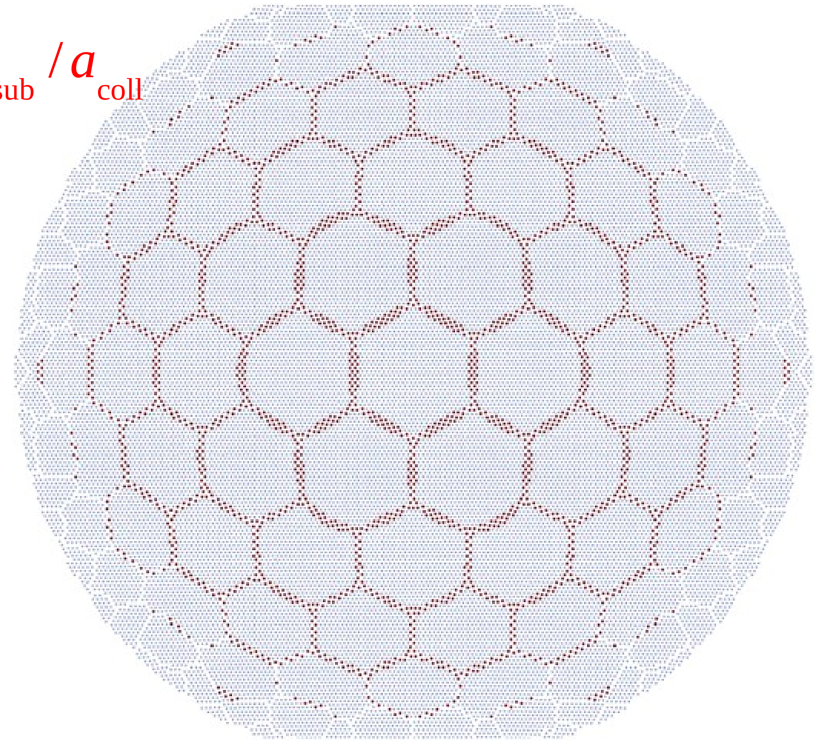


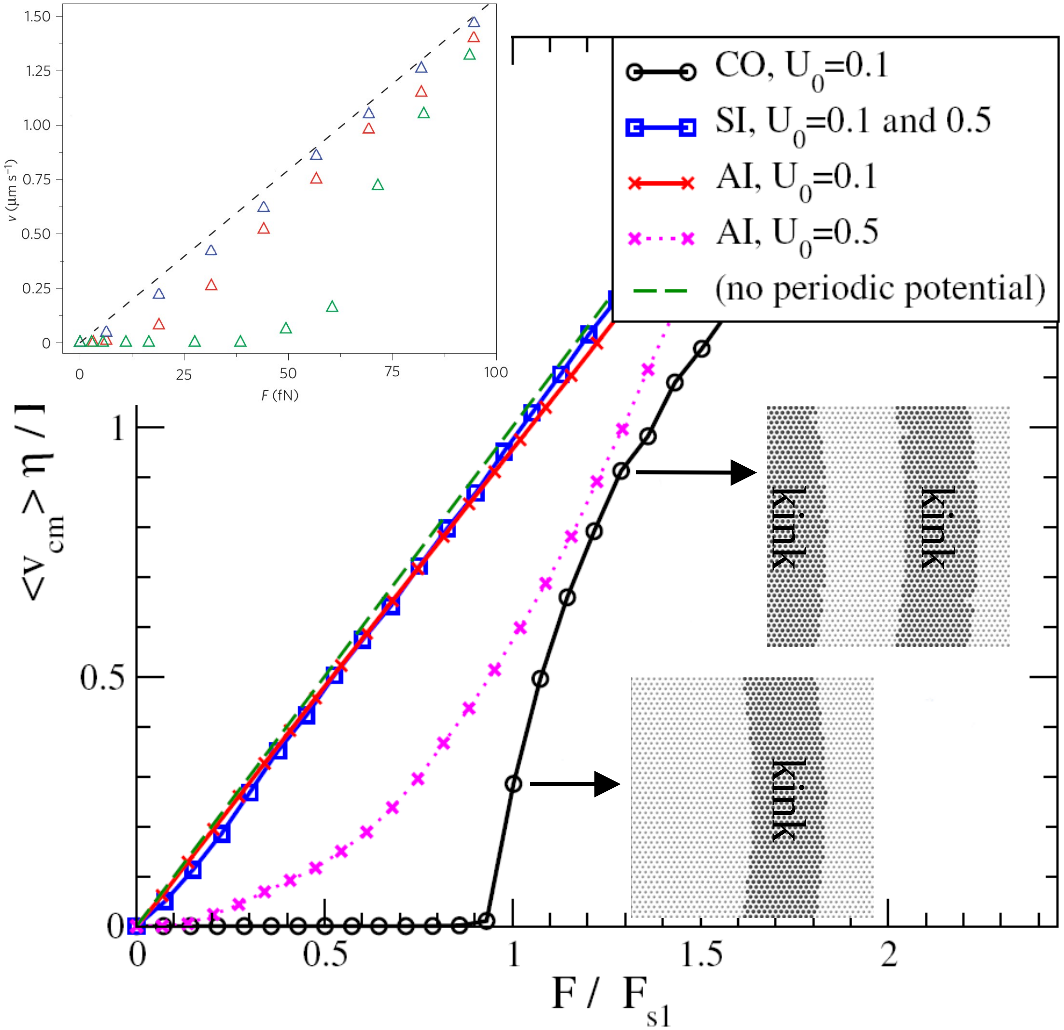
  - 3 representative cases:
    - underdense, $\rho = 0.95$ (AI)
    - nearly commensurate, $\rho \simeq 1.0$ (CO)
    - overdense, $\rho = 1.05$ (SI)

- In order to:
  - mimic the experiment,
  - prevent solitons from leaving the finite-size sample,

the external force F is ramped adiabatically alternating in sign (back and forth).

MD results

force-velocity characteristics



- ***large static friction force*** for $\rho \simeq 1$ CO
- for ***moderate corrugation*** U_0 ***and 5% lattice mismatch***, static friction drops essentially to zero, and a nearly free viscous sliding is realized (***superlubricity***)
- by ***increasing*** U_0, the AI mobility drops to zero at small force, and ***pinning reemerges despite AI*** incommensurability
- by contrast, ***SI configurations remain superlubric*** up to much larger U_0.

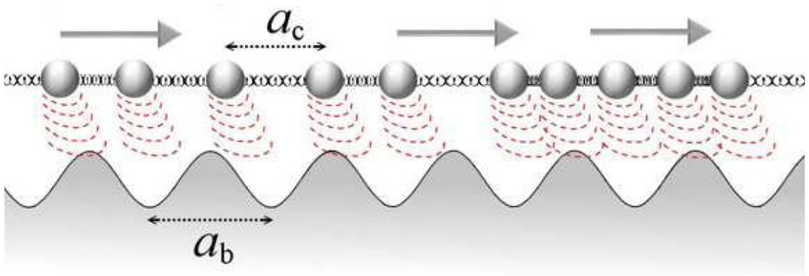
- snapshots of the central region of the initially commensurate colloid during motion, illustrating sliding-generated solitons, whose density increases as F is increased.

Note: colloids located at repulsive spots of the corrugation potential [$W(r) > -U_0/2$] are drawn as dark points, while colloids nearer to potential minima [$W(r) \leq -U_0/2$] are light.

Vanossi, Manini, Tosatti, PNAS 109, 16429 (2012).

General theory: recall the Aubry transition

- The *1D Frenekel-Kontorova model*, *harmonically interacting atoms subject to a sinusoidal potential*



$$H = \frac{m}{2}\sum_i \dot{x}_i^2 + \sum_i \left[\frac{K}{2}(x_{i+1} - x_i - a_c)^2 + \frac{\mathcal{E}}{2}\left(1 - \cos\frac{2\pi}{a_b}x_i\right)\right],$$

undergoes, for *incommensurate configurations* (a_b/a_c ***irrational***) and fixing the amplitude ε, the famous ***Aubry transition*** at a critical value K_C of the interatomic interaction.

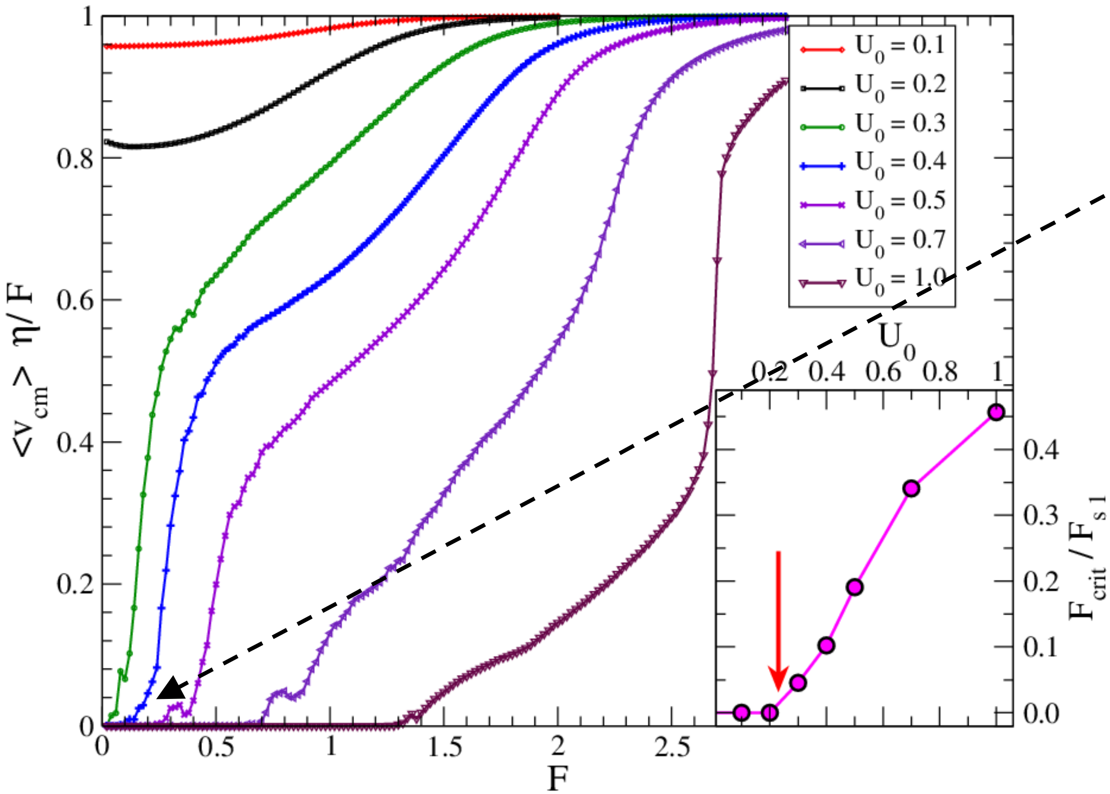
Above the transition $(K > K_C)$	*Below the transition* $(K < K_C)$
▸ no forbidden regions over the substrate potential for the values x_i	▸ particles trapped close to the minima of the substrate potential, forbidden regions arise
▸ incommensurate ground states described by an analytic hull function	▸ incommensurate ground states described by a non-analytic hull function
▸ zero static friction *(superlubricity)*	▸ finite static friction *(pinning)*

Peyrard and Aubry, J. Phys. C: Solid State Phys. 16, 1593 (1983).
Braun and Kivshar, The Frenkel-Kontorova Model (Springer, Berlin, 2004).
Vanossi and Braun, J. Phys.: Condens. Matter 19, 305017 (2007).

MD results: the Aubry transition

Even in our 2D case, it is expected that incommensurate colloids, underdense ($\rho \lessapprox 1$) or overdense ($\rho \gtrapprox 1$), undergo an Aubry-like superlubric-to-pinned transition for increasing U_0.

mobility vs applied force for ρ = 0.95 (AI) [infinite-size colloid system]



appearance of pinning just above U_0 = 0.2

normalized static friction F_{crit} vs U_0 the arrow indicating the critical Aubry corrugation

This ***ρ-dependent critical U_0*** is ***much larger for overdense SI*** than for underdense AI colloids

The ***soliton-antisoliton asymmetry*** arises from the intercolloid effective spring constant

$$\frac{V''(a \pm \delta)}{V''(a)} \simeq \exp(-\delta/\lambda_D)$$

Vanossi, Manini, Tosatti, PNAS 109, 16429 (2012).

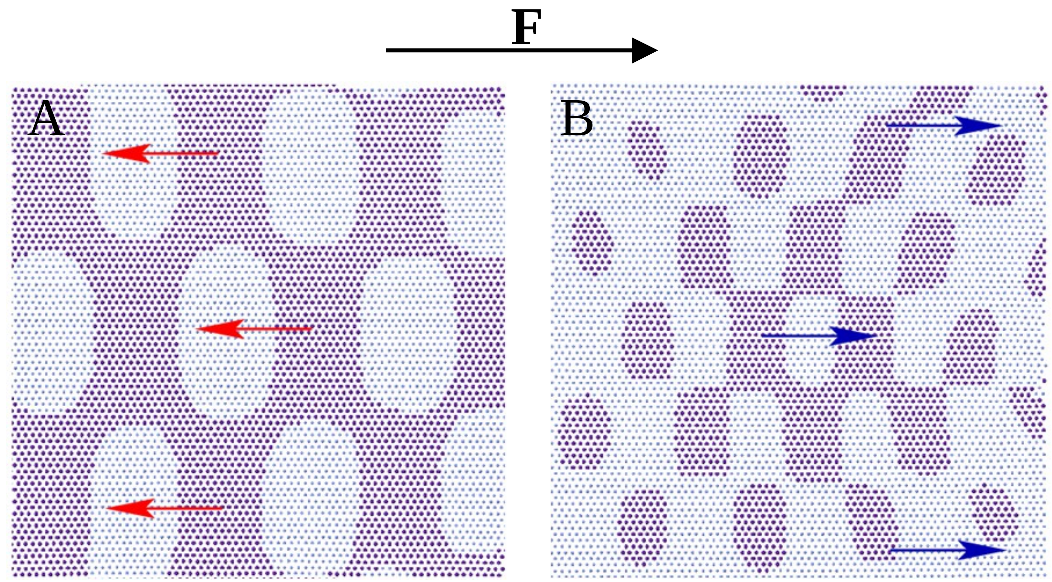
MD results

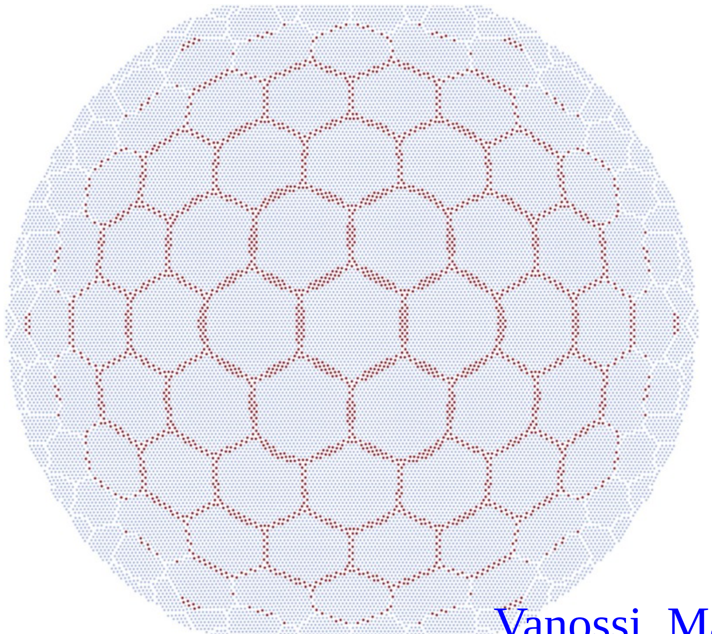
incommensurate colloid: sliding states

- The evolution of solitons/antisolitons (comparable with experiment) is of immediate interest. With increasing F, their arrangements elongate into a stripe-like pattern perpendicular to the driving direction.

(A) For underdense colloid (ρ = 0.95), preformed antisolitons fly backward antiparallel to the rightward force.

(B) For overdense colloid (ρ = 1.05), preformed solitons fly rightward, parallel to the force.





Dropping the back-and-forth driving protocol,

- antisolitons are eventually absorbed at the left edge boundary, while new ones spawn at the right edge, sustaining a steady-state mobility;

- solitons instead are not automatically spawned at the boundary, owing to the decreasing density.

Vanossi, Manini, Tosatti, PNAS 109, 16429 (2012).

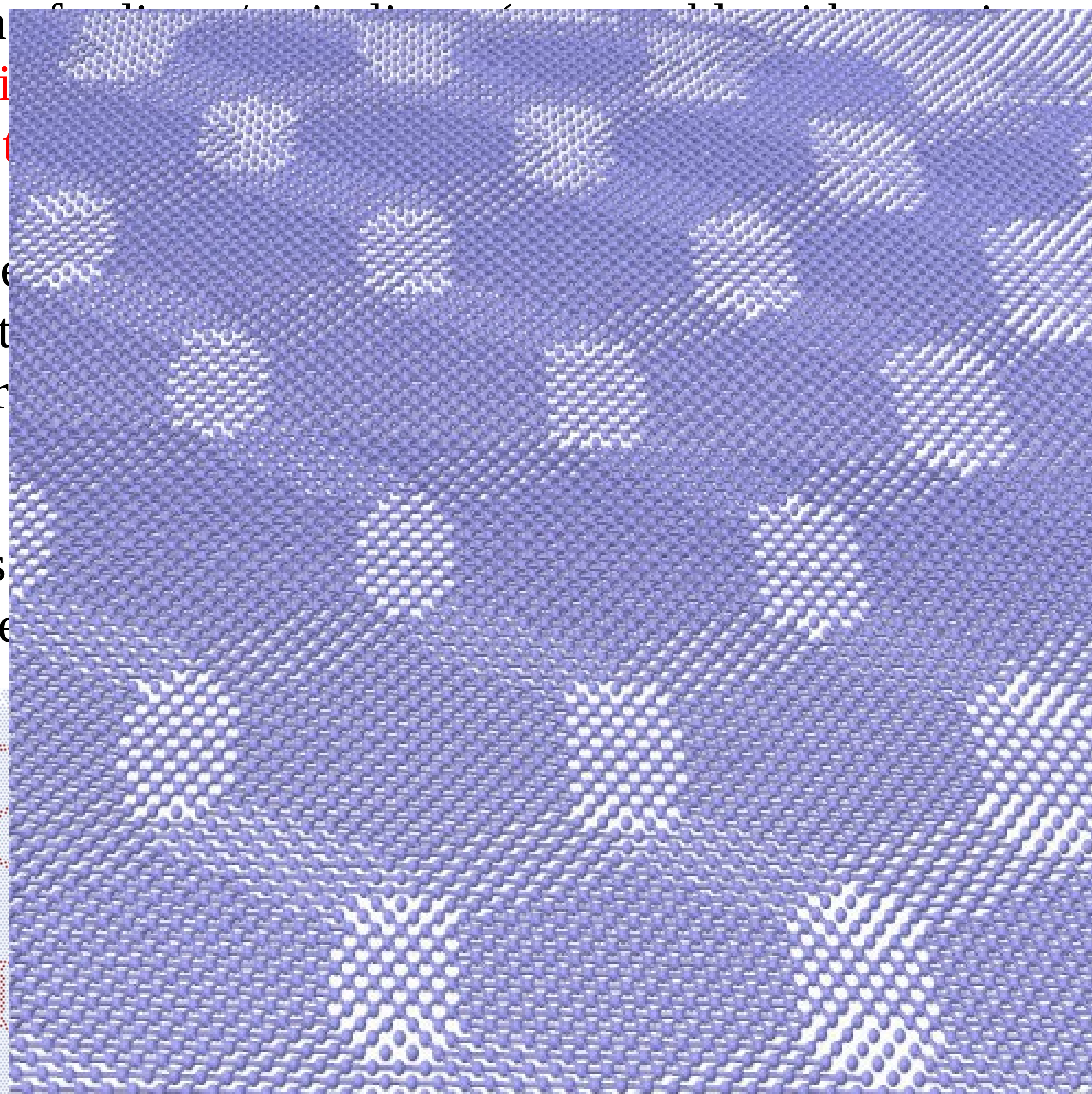
MD results

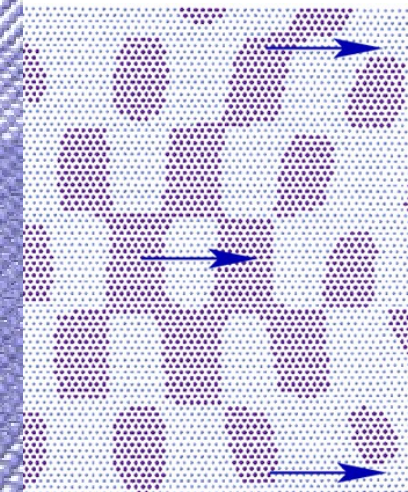
incommensurate colloid: sliding states

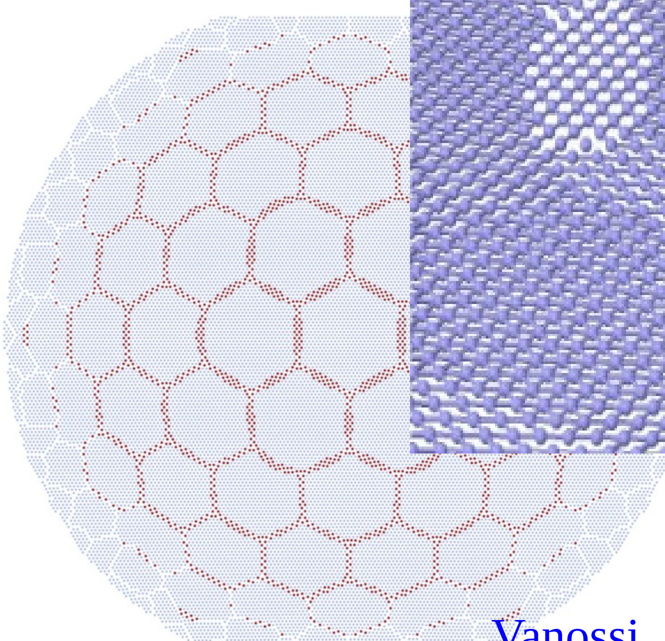
- The evolution) is of immediate interest. With i like pattern perpendicular t

(A) For underdense preformed antisolit antiparallel to the r

(B) For overdense preformed solitons parallel to the force







otocol,

the left edge

right edge,

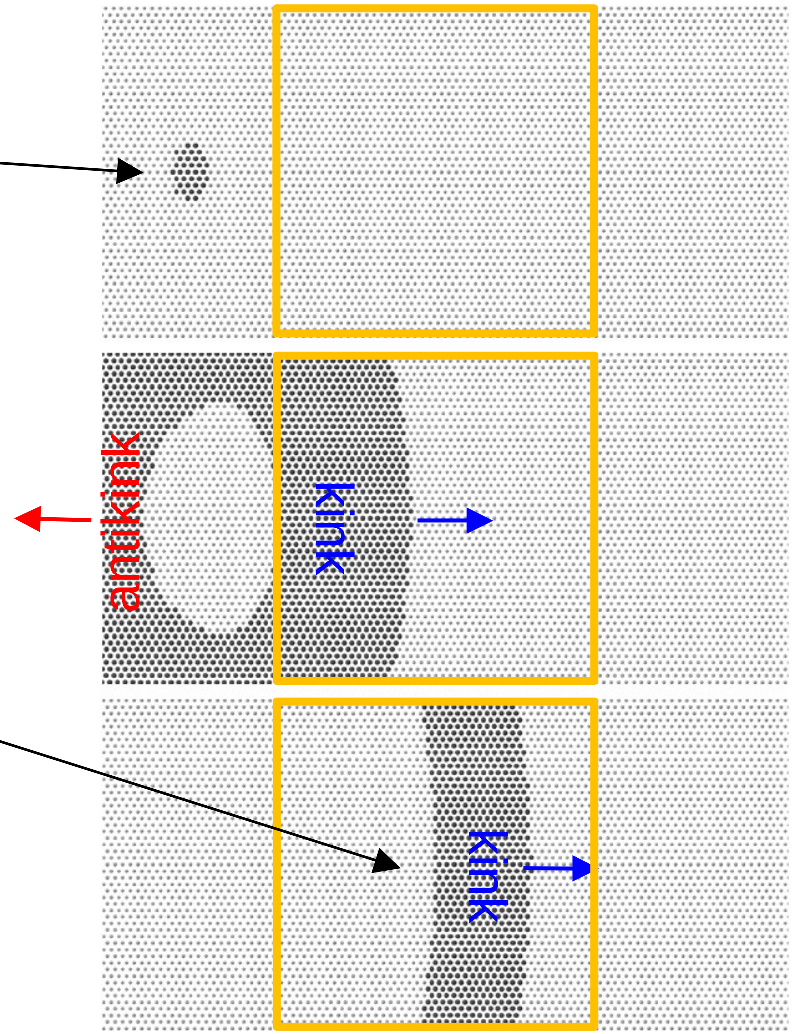
- solitons instead are not automatically spawned at the boundary, owing to the decreasing density.

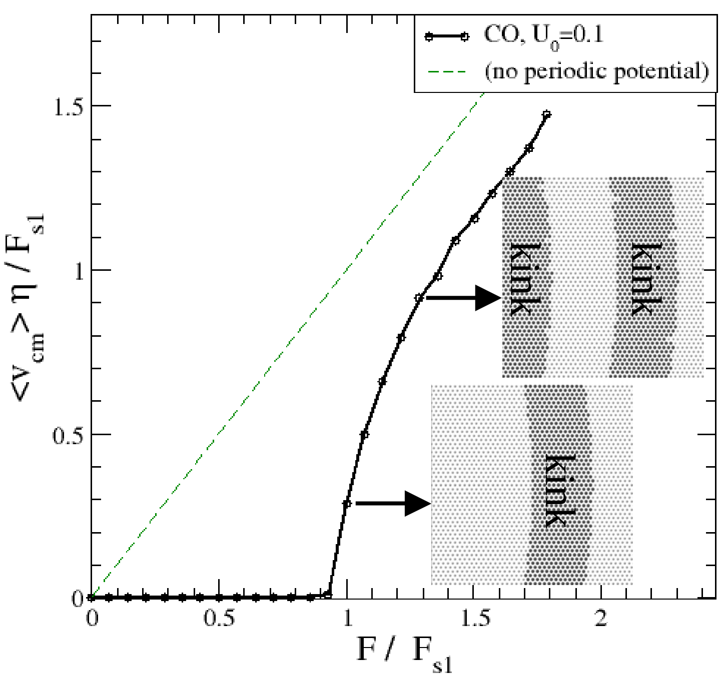
Vanossi, Manini, Tosatti, PNAS 109, 16429 (2012).

MD results

commensurate colloid: sliding states

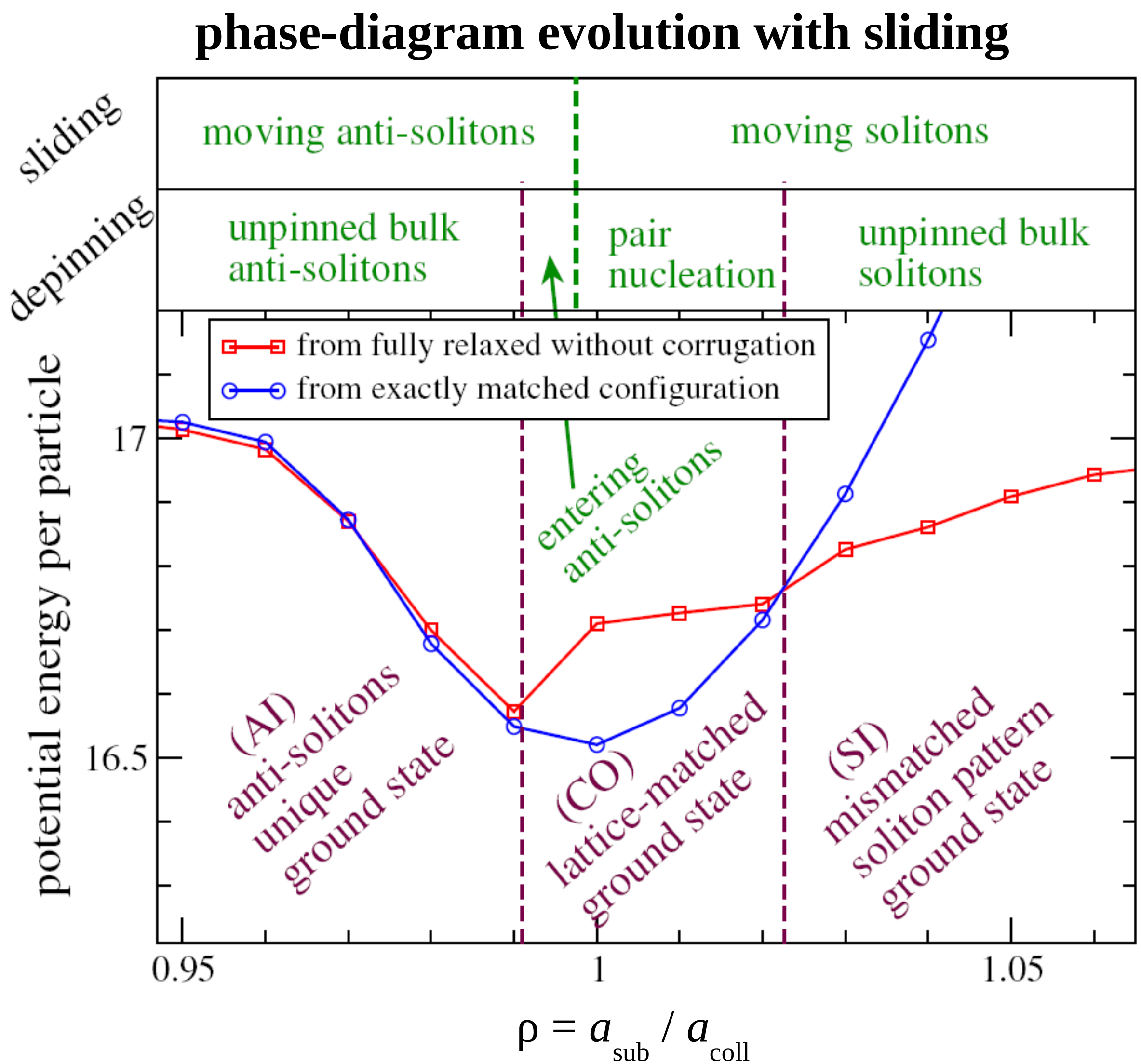
- the colloid only moves after static friction is overcome
- motion initiates by nucleation of soliton–antisoliton pairs inside the bulk -close to the left edge because the central region tends to be slightly overdense
- antisolitons flow leftwards and become undetectable to the optically monitored central part of the colloid, where only solitons transit, as seen in experiment





- for pinned CO colloid the soliton density, initially zero, actually increases with increasing driving force

MD results



- With a nominal $\rho \approx 1$, but not exactly commensurate, the monolayer can realize (depending on U_0) a static arrangement with fully lattice-matched CO state.

- Under the external force, sliding may tilt the balance in favor of the 'natural' slightly mismatched arrangement, populating the former static CO phase with solitonic structures.

MD results

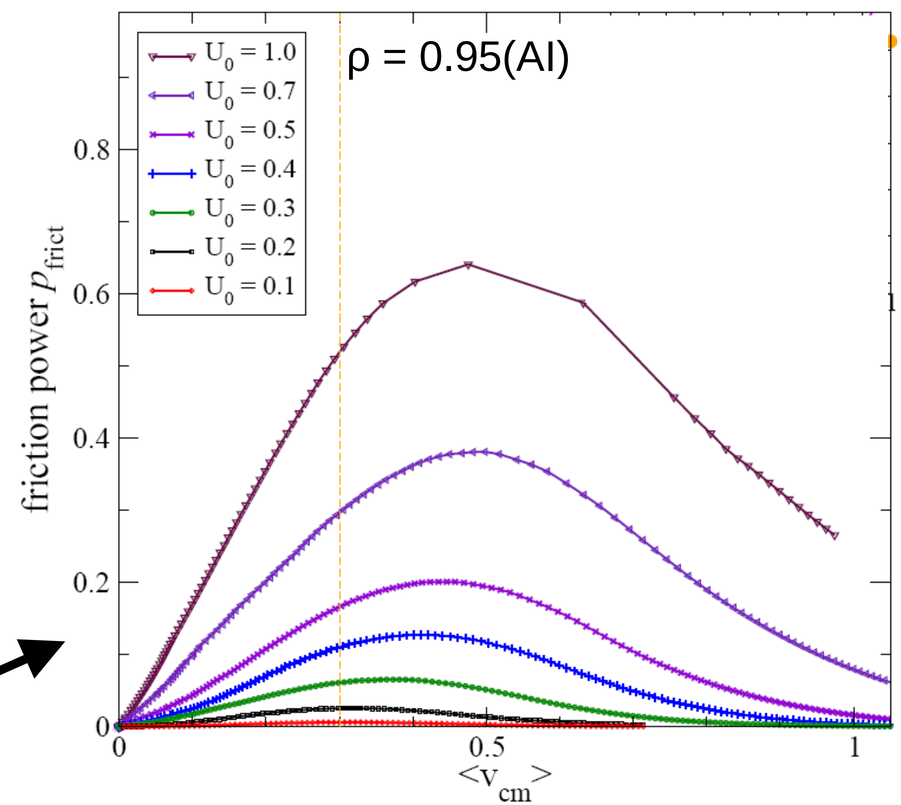
- Under steady sliding, the time-averaged overall power balance

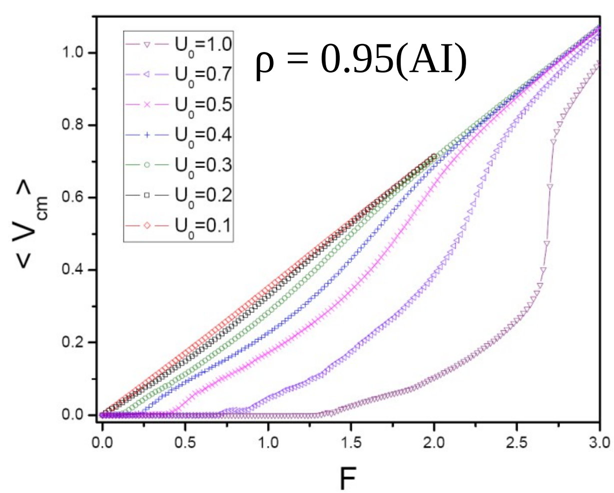
$$
\begin{aligned}
P_{\text{tot}} &= \sum_i \eta \langle (\mathbf{v}_d - \mathbf{v}_i) \cdot \mathbf{v}_i \rangle \\
&= \left(N\mathbf{F} \cdot \langle \mathbf{v}_{\text{cm}} \rangle - \eta \langle |\mathbf{v}_{\text{cm}}|^2 \rangle \right) - \eta \sum_i \langle |\mathbf{u}_i|^2 \rangle \\
&= P_{\text{frict}} - P_{\text{kin}}, \qquad\qquad (\mathbf{u}_i = \mathbf{v}_i - \mathbf{v}_{\text{cm}})
\end{aligned}
$$

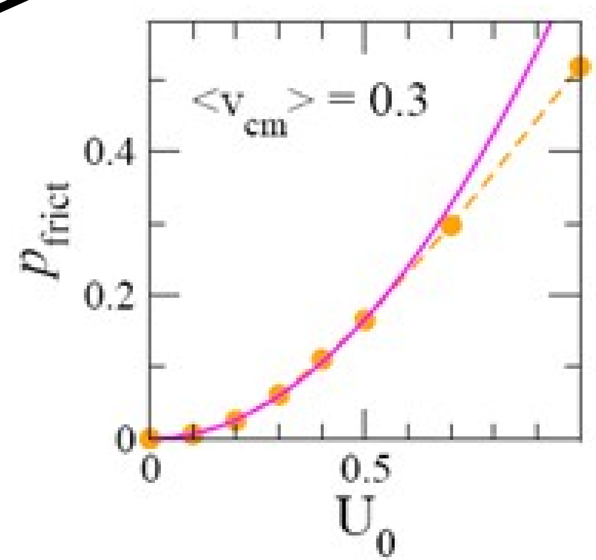
vanishes ($P_{\text{tot}} = 0$), and the effective friction power is exactly balanced by an internal kinetic energy excess rate.

$$
p_{\text{frict}} = \frac{P_{\text{frict}}}{N} \simeq \mathbf{F} \cdot \langle \mathbf{v}_{\text{cm}} \rangle - \eta |\langle \mathbf{v}_{\text{cm}} \rangle|^2
$$

friction dissipation





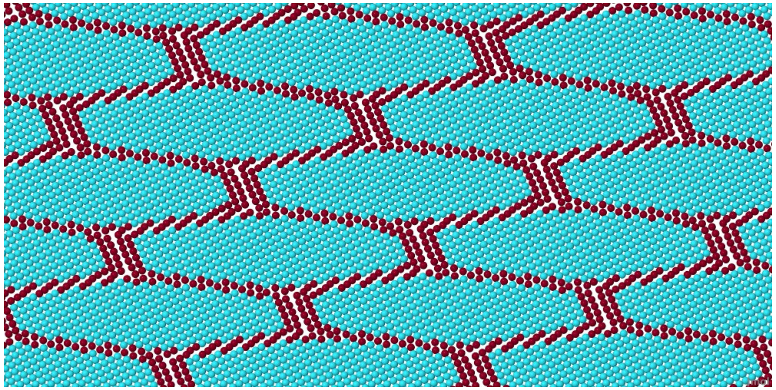


friction increase with U_0, for a chosen speed, is found quadratic at weak corrugation, gradually turning to linear for larger U_0 values

Summary

Driven colloid systems offers the attractive possibility:

- to change parameters (symmetries, lattice spacings, corrugation amplitudes) freely
- to compare directly experiment with simulations, testing theoretical predictions
- to visualize in real-time in simple cases the intimate mechanisms of sliding friction, relating the overall tribological response to the detailed particle dynamics



Outlook

This work opens several lines of present & future research:

- trapping-and-driving method to introduce stick-slip
- friction tuning by oscillating substrate potentials
- dependence of friction on contact size
- sliding on peculiar substrate geometries
- large colloidal crystal sizes to address mesoscopic complexity

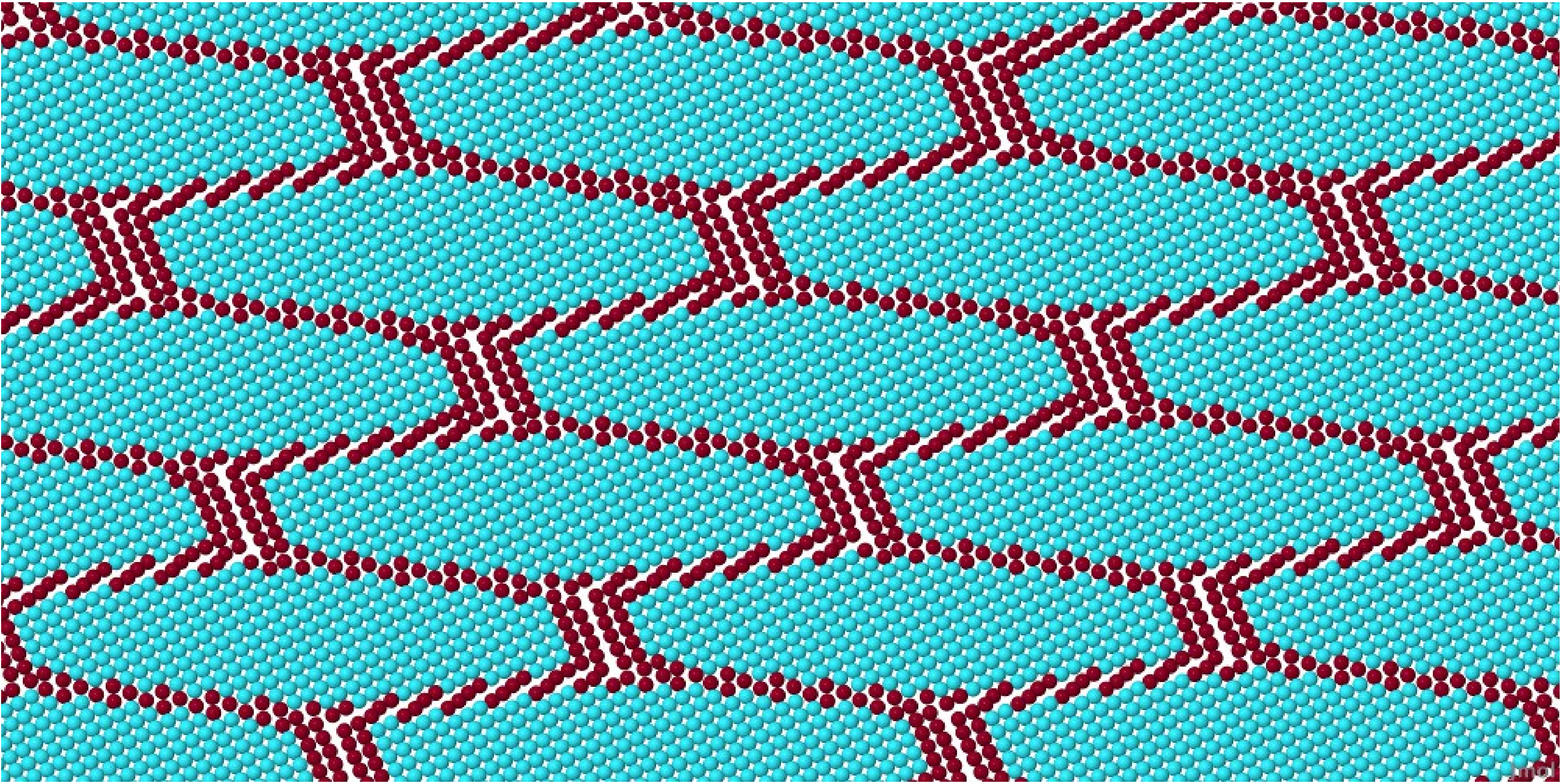


Table S2. Basic units for various quantities in our model, with typical values appropriate for the setup by Bohlein et al. 1.

Physical quantity	Model expression	Typical value
Length	a_{coll}	5.7 μm
Force	$F_0 = 9F_{s1}/(8\pi)$	18 fN
Viscosity coefficient	η	6.3×10^{-8} kg/s
Energy	$F_0 a_{\mathrm{coll}}$	1.0×10^{-19} J
Time	$\eta a_{\mathrm{coll}}^2/U_0$	20 s
Mass	$\eta^2 a_{\mathrm{coll}}/F_0$	1.3×10^{-6} kg
Velocity	F_0/η	0.284 μm/s
Power	F_0^2/η	5.1×10^{-21} W

Table S3. Numerical parameters adopted in the simulation, Eqs. S3, S5, S6, and S7, expressed in model units, to be scaled according to Table S2. L_x and L_y are the sides of the rectangular simulation supercell, respectively.

	η	N	Q	λ_D	A_c	σ	n	U_0	L_x	L_y
Cluster	1.4	28,861	10^{13}	0.03	1,200	1,200	3	0.1	500	500
Bulk	1.4	28,080	10^{13}	0.03	0.0	1,200	3	0.1	156	$90\sqrt{3}$