Novaco-angle
investigation of friction
in a colloidal monolayer
on a quasicrystalline substrate

Relatore: Prof. Nicola Manini
Correlatore: Dr. Andrea Vanossi

Alex Raiteri
Matricola n° 886157
A.A. 2018/2019

Codice PACS: 61.44.-n
Novaco-angle investigation of friction in a colloidal monolayer on a quasicrystalline substrate

Alex Raiteri
Dipartimento di Fisica, Università degli Studi di Milano,
Via Celoria 16, 20133 Milano, Italia

December 12, 2019

Abstract

We investigate the frictional properties of a colloidal layer interacting with an external corrugation potential characterized by five-fold quasicrystalline symmetry. We first investigate the energetics, identifying the lowest-energy configuration by comparing our simulations with a generalization of the Novaco-McTague theory of orientational epitaxy. We then proceed to drive the colloidal overlayer, identifying a static-friction depinning transition and its disappearance in favor of a superlubric sliding for weak corrugation.

Advisor: Prof. Nicola Manini
Co-Advisor: Dr. Andrea Vanossi
# Contents

1. Introduction .................................................. 3

2. The model .................................................... 4
   2.1 Interactions ........................................... 4
   2.2 Colloidal monolayer .................................. 6
   2.3 Novaco-McTague theory ................................ 7

3. Technical implementation .................................. 7
   3.1 The FIRE Algorithm .................................. 8
   3.2 Supercell .............................................. 8
   3.3 Initial Condition and Mismatch ..................... 9
   3.4 Construction of the relaxed initial configuration . 10

4. Results ..................................................... 10
   4.1 Validity range ........................................ 10
   4.2 Comparison between theory and simulation .......... 13
   4.3 Dynamics .............................................. 13

5. Discussion and Conclusion ................................ 16

References ..................................................... 19
1 Introduction

Tribology is the science that studies the relative motion of interacting surfaces, one of its main subject matter is friction. Many different phenomena such as earthquakes, wear or crack propagation are related to friction between solids. Macroscopic objects only touch each other locally because of their surface roughness. Conversely, atomically flat surfaces form spatially extended contacts. Considering a flat monolayer of interacting particle on a periodic potential substrate the Frenkel-Kontororova model has been used to described such contact. This model for mismatched periodicities predicts the presence of solitons or antisolitons \cite{1}, which reduce friction significantly. These excitations dominate the frictional properties because they supply an efficient mechanism for mass transport.

One of the main experimental difficulties is the impossibility of observe directly the motion of the considered bodies. This difficulty is circumvented in experiments done with layer of colloids, which are visible under the microscope. Solitons and antisolitons were observed in the pioneering experiment by T. Bohlein, J. Mikhael and C. Bechinger, who investigated the frictional properties of a colloidal monolayer driven across a periodic or quasiperiodic potential \cite{2}. They observed a dissipative stick-slip motion for commensurate conditions, while for incommensurate conditions they noticed a superlubric regime, where the friction coefficient vanished. A computational reproduction of this results \cite{3} characterized the presence of the superlubric regime depending on the corrugation amplitude. This dependence gives rise to an Aubry transition, namely a transition between superlubric and pinned states, the latter being characterized by the presence of static friction.

In this work we consider a colloidal monolayer on a quasiperiodic potential substrate and we investigate its energetic and frictional properties. A quasiperiodic potential is characterized by long range order without being periodic. In this thesis we consider a five-fold symmetry potential generated by the interference of five laser beams. The colloidal monolayer is composed of micrometer-size charged particles. The orientational hepitaxy of a monoatomic layer has been studied by A. D. Novaco and J. P. McTague \cite{4, 5}. There an energy dependence was demonstrated on the relative angle between the hepitaxial layer and the substrate corrugation potential. The validity of the NM theory is restricted for a weak interaction between the overlayer and the substrate. The same physics has been discovered in colloidal layer interacting with a periodic external potential \cite{6}, and observed experimentally in the same context \cite{7}.

The similar misalignment in the quasiperiodic case is challenging \cite{8}, and it remains an open problem. Our first goal is to define the range in which we
can generalized the Novaco-McTague (NM) theory, then compare this prediction with our minimization, done by means of the FIRE algorithm. Once we identify the minimum energy configuration, it is interesting to study friction in such unconventional setup.

2 The model

In our model we consider a colloidal monolayer moving in a fluid and interacting with a quasiperiodic potential substrate shown in Fig. 1.

Our colloid is a 2D layer composed of charged particles, with diameters close to 4 µm, suspended in a fluid. We treat the colloids as charged point-like particles because the colloids interaction keeps the distance between their centers well above their diameters. The colloids form a 2D layer, because the gravity pushes them down onto a flat surface.

2.1 Interactions

The interactions considered in our model are between the colloids, with the external potential corrugation and with the fluid.
The interaction between colloids are given by a two-body potential:

\[ U_{cc} = \frac{1}{2} \sum_{j \neq l}^{N} U_{2B}(r_{j,l}). \]  

(1)

In Eq.(1), \( r_{j,l} = |r_j - r_l| \) is the inter-colloid distance and \( U_{2B} \) is the Yukawa potential:

\[ U_{2B}(r) = \frac{Q}{r} \exp \left( \frac{-r}{\lambda} \right), \]  

(2)

where \( Q \) is the coupling strength and \( \lambda \) is the Debye screening length. Due to computational limit we impose a cutoff, a maximum distance \( r_{\text{cut}} \) above which the potential is identically null. To avoid abrupt jumps in the potential and force passing \( r_{\text{cut}} \) we set the potential and its derivative to zero at \( r_{\text{cut}} \) by adding to the potential in Eq.(2) a linear function as described in Ref.[9].

The quasiperiodic substrate potential \( U_{\text{ext}} \) can be generated by the interference of five laser fields. The general form of a sum of \( n \) coherent laser fields is given by:

\[ W(r) = - \frac{V_0}{n^2} \left| \sum_{l=0}^{n-1} e^{i k_l \cdot r} \right|^2 = - \frac{V_0}{n^2} \sum_{j,m=0}^{n-1} e^{i G_{m,j} \cdot r}, \]  

(3)

where \( k_l \) is the in-phase component wave vector of the electromagnetic wave and \( V_0 \) is the potential amplitude. In the last equality we introduce:

\[ G_{m,j} = k_m - k_j. \]  

(4)

We take \( n = 5 \) that gives us 20 different \( G_{m,j} \). We take the five laser with the same phase so that their wave vectors can be chosen as:

\[ k_l = \frac{2\pi}{a_{\text{coll}}} \left( \cos \frac{2\pi(m-1)}{5}, \sin \frac{2\pi(m-1)}{5} \right). \]  

(5)

The motion of the \( n \)-th colloid then follows the equation:

\[ m_{\text{coll}} \ddot{r}_n + m_{\text{coll}} \eta (\dot{r}_n - v_d \hat{x}) = -\nabla_{r_n} (U_{2B} + U_{\text{ext}}). \]  

(6)

The colloids interacts also with the fluid: this interaction gives a dissipative term represented in Eq.(6) by the viscous damping term proportional to \( \eta \).

\( v_d = v_d \cdot u_x \) is the drift velocity of the fluid, which can be used to generate a uniform Stokes driving force \( F = m_{\text{coll}} \eta v_d \) acting on the colloids.
2.2 Colloidal monolayer

The colloidal monolayer corresponds to a bi-dimensional hexagonal Bravais lattice, whose unit vectors are:

\[ a_1 = \text{coll} \hat{u}_x \]

\[ a_2 = \frac{\text{coll}}{2} \hat{u}_x + \frac{\sqrt{3} \text{coll}}{2} \hat{u}_y. \]

The primitive vectors of the reciprocal lattice, \( b_i \), is defined by the relation : \( b_i \cdot a_j = 2\pi \delta_{i,j} \), or in the matrix notation:

\[
\begin{pmatrix}
 b_{1,x} & b_{1,y} \\
 b_{2,x} & b_{2,y}
\end{pmatrix}
\cdot
\begin{pmatrix}
 a_{1,x} & a_{2,x} \\
 a_{1,y} & a_{2,y}
\end{pmatrix}
= 2\pi \begin{pmatrix}
 1 & 0 \\
 0 & 1
\end{pmatrix},
\]

and multiplying at the right by the inverse of the matrix with \( a_{i,j} \) component we end up with:

\[ b_1 = \frac{2\pi}{\text{coll}} \left( \hat{u}_x - \frac{1}{\sqrt{3}} \hat{u}_y \right) \]

\[ b_2 = \frac{4\pi}{\text{coll} \sqrt{3}} \hat{u}_y. \]

We denote with \( \tau \) a general vector of the reciprocal lattice:

\[ \tau = \sum_{i=1}^{2} l_i b_i. \]
2.3 Novaco-McTague theory

From the NM theory of Ref.[5], using the harmonic approximation for the interaction between colloids and taking the one-phonon approximation we end up writing the energy per colloid as:

\[
\epsilon_{1-ph} = -\frac{V_0^2}{2m_{coll}} \sum_{q} \sum_{s=L,T} \omega_{q,s}^2 |f_{q,s}|^2 \tag{13}
\]

\[
f_{q,s} = \sum_{G_{m,j}} \sum_{\tau} G_{m,j} \cdot \epsilon_{q,s} \exp(-i\tau \cdot R_0) \delta(q(G_{m,j}-\tau)), \tag{14}
\]

where \(V_0\) is the potential amplitude, \(m_{coll}\) is the colloid mass, \(R_0\) is the origin of the lattice, \(q\) are the wave vectors associated with the displacements from the equilibrium position, \(G_{m,j}\) and \(\tau\) were introduced respectively in Eq.(4) and Eq.(12). \(\omega_{q,s}\) is the frequency related to the harmonic vibration, \(s = L, T\) label the longitudinal and transverse modes of vibration of the free \((V_0 = 0 zJ)\) monolayer, \(\epsilon_{q,s}\) are the eigenvectors (polarization vectors) for these vibration. They form as usual an orthonormal set:

\[
\epsilon_{q,s} \cdot \epsilon_{q,s'} = \delta_{s,s'}, \tag{15}
\]

In the limit of small \(|q|\) the following approximation holds:

\[
\omega_{q,s} \simeq c_s |q|, \tag{16}
\]

where \(c_s\) are the monolayer sound velocities. Following the procedure of Ref.[12] we find for our system the values \(c_L = 0.3762\) mm/s and \(c_T = 0.2072\) mm/s.

The coupling between the 10-fold symmetry of \(G_{m,j}\) (that are 20 but come in pairs of opposites) and the hexagonal lattice gives rise to a 12° symmetry in the total energy per particle. Moreover, due to the inversion symmetry \(\theta \rightarrow -\theta\), we end up with a 6° range where it is necessary to investigate the energetics. The entire 360° range can be reconstructed based on these 6°, using symmetry.

3 Technical implementation

Our simulations are executed by means of a molecular-dynamics computer code written in fortran90. By default, it integrates the equations of motion, by means of a Runge-Kutta algorithm, but it can also execute minimization by means of an implementation of the FIRE algorithm.
3.1 The FIRE Algorithm

FIRE (Fast Inertial Relaxation Engine) is an algorithm used for finding mechanically stable equilibrium configurations of atomistic systems, well described in Ref.[10]. It is based on a discrete form of the equation:

\[
\dot{v}(t) = \frac{F(t)}{m} - \gamma(t)|v(t)| \left( \dot{v}(t) - \hat{F}(t) \right),
\]

(17)

where \(m\) is the mass, \(v = \dot{x}\) is the velocity and \(F\) is the force. The final term at the right side of Eq.(17) is added to the standard equation of motion, and allows to introduce an acceleration in a direction that is steeper than the current direction of motion, via \(\gamma\), when the power \(P = F(t) \cdot v(t)\) is positive, and stop the velocity to avoid uphill motion as soon as the power becomes negative. FIRE can be based on any Molecular Dynamics (MD) method, the latter is based on the integration of the equation of motion with fixed time step \(\Delta t\). Practically the FIRE algorithm performs the following cycle:

- \(x, F\) and \(v\) are calculated using a common MD integrator. Then evaluate \(P = F \cdot v\), set \(v \rightarrow (1 - \alpha) \cdot v + \alpha \cdot \hat{F} \cdot |v|\), resulting from an Euler discretization of the second term on the right side of Eq.(17). Then we can have two possible scenarios. In the first one, \(P\) stays positive for a number of steps larger than \(N_{\text{min}}\), then increase the time step \(\Delta t \rightarrow \min(\Delta t \cdot f_{\text{inc}}, \Delta t_{\text{max}})\) and decrease \(\alpha \rightarrow \alpha f_{\alpha}\).
- In the second scenario \(P\) is negative or zero, the velocity stops, the time step decrease \(\Delta t \rightarrow \Delta t \cdot f_{\text{dec}}\) and \(\alpha\) is set back to \(\alpha_{\text{start}}\). Then return to MD. Referring again to Ref.[10] we use the following values for the parameters: \(N_{\text{min}} = 5\), \(f_{\text{inc}} = 1.1\), \(f_{\text{dec}} = 0.5\), \(\alpha_{\text{start}} = 0.1\), \(f_{\alpha} = 0.99\) and \(\Delta t_{\text{max}} = 10 \Delta t_{\text{MD}}\), where \(\Delta t_{\text{MD}}\) may also be larger than the typical MD simulation time step, in our case we use \(\Delta t_{\text{MD}} = 100 \mu s\).

3.2 Supercell

The colloids are simulated in a supercell with periodic boundary conditions (PBC) to solve the problem of being able to consider only a finite number of colloids but at the same time mimicking the presence of an infinite lattice at fixed density. We did it in the simplest way (see Fig.3): the supercell has the same shape as the unit cell and primitive vectors that are integer multiples of the unit vectors in Eq.(7) and Eq.(8):

\[
b_1 = Na_1
\]

(18)

\[
b_2 = Na_2
\]

(19)
Figure 3: Blue: the two supercell primitive vectors. Red: the colloids arranged as hexagonal Bravais lattice. Green: supercell boundary. Here $N = 10$.

Were $N$ is an integer to satisfy the periodic boundary condition. To comply with the PBC we must include only one side for each pair of opposite sides on the boundary.

3.3 Initial Condition and Mismatch

In the choice of the parameters, we follow Refs.[8,11], in particular we fix $a_{coll} = 5.8 \, \mu m$ for the particles lattice spacing, $m_{coll}=31.0593557697 \, \text{fkg}$ for the mass of the colloids, $Q = 10^{11} \, \text{zJ} \, \mu m$ and $\lambda = 0.2 \, \mu m$ to defined the colloid-colloid

<table>
<thead>
<tr>
<th>Physical quantity</th>
<th>value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_{coll}$</td>
<td>5.8 $\mu m$</td>
</tr>
<tr>
<td>$Q$</td>
<td>$10^{11} , \text{zJ} , \mu m$</td>
</tr>
<tr>
<td>$\lambda_D$</td>
<td>0.2 $\mu m$</td>
</tr>
<tr>
<td>$r_c$</td>
<td>10 $\mu m$</td>
</tr>
<tr>
<td>$N_{coll}$</td>
<td>10 000 or 40 000</td>
</tr>
<tr>
<td>$m_{coll}$</td>
<td>31.0593557697 fkg</td>
</tr>
</tbody>
</table>

Table 1: Parameters used in the simulations.
screened Coulomb interaction, with a cutoff $r_c = 10 \, \mu m$.

For all the simulations we take a supercell with vectors $b_1 = N \mathbf{a}_1$ and $b_2 = N \mathbf{a}_2$, including a total of $N^2 = 10000$ or 40000 colloids. We focus our studies on the case $a_{pot} = 5.2 \, \mu m$, a slightly underdense case in which we have approximately one colloid per potential well.

### 3.4 Construction of the relaxed initial configuration

The simulations of friction require an initial colloid configuration that minimizes energy at least locally. We use the FIRE algorithm introduced in Sec. 3.1. We observe that in addition to a relative rearrangement of the colloids every minimization implies an almost rigid translation of the center of mass. This is consistent with the NM theory, which can tell us nothing about a rigid translation by $R_0$. This energy lowering is, however, too small even for the fire algorithm and this implies impractical simulation times before reaching the global minimum. We have observed, however, that this translation of the center of mass seems to drive it toward the origin. Thus we rigidly shift the center of mass to the origin, leading rapidly very close to the minimum. For this reason we start all our relaxations with the monolayer center of mass translated to the origin.

The only variables that can be varied between one simulation and another are the starting configuration, the relative rotation between the substrate and the adsorbate, the starting time step $\Delta t$ and the maximum number of step $n_{max}$. Furthermore there are two additional parameter that can be set to stop the simulation before reaching $n_{max}$: a force and an energy threshold. In particular the first one imposes a limit on the minimum total force acting on the colloids, below which the simulation stops, the second one imposes a limit on the difference of the total energy between one step and the previous.

The typical values for $\Delta t$ and $n_{max}$ in our FIRE minimizations are respectively 100 $\mu s$ and 5000 steps. We set a severe energy threshold that imposes a relative energy difference $|\delta E|/E \leq 10^{-16}$, to the last significant digit. We set the force limit at $10^{-10}$ N, but this never stops our minimization.

### 4 Results

#### 4.1 Validity range

In order to evaluate the validity range of the NM theory we need to find the relation between the total energy lowering and the square of the potential amplitude $V_0^2$. To do so we start from a minimization at a potential amplitude of 0.01 zJ and
find the optimal displacements of the colloids at the minimum energy. Then we start two series of simulation increasing up to 10 zJ and down to $10^{-4}$ zJ, starting the new simulation with the final configuration of the previous one: this help us to reduce the computational time, we expect in fact that the final configuration of two successive simulations with similar $V_0$ will not vary much.

Figure 4 shows the minimization data and the line obtained fitting the data points in the range $V_0 = 10^{-3} - 10^{-2}$ zJ with a this simple power law: $-\Delta E_{tot} = AV_0^2$. For the smaller potential amplitudes considered, of magnitude $V_0 = 10^{-4}$ zJ, we observe a deviation of the data from the fitted line. We will discuss this small relative-$V_0$ deviation below.

At amplitudes above approximately $V_0 = 0.05$ zJ we see that the data deviate from the fitted line moving above it for a small range, approximately $V_0 = 0.05$ zJ : 0.4 zJ and above $V_0 \simeq 0.4$ zJ moving below the linear-response line and deviate more and more from it. This is the range where nonlinearity sets in. We can check this by plotting separately the two contributions to the total energy lowering.

A prediction of the NM theory is that the contributions of the energy low-
Figure 5: Log-log scale plot of the total energy difference as in Fig. 4 and its contributions from the colloid-colloid and colloids-substrate interaction, respectively in blue, green and red. To better compare them we change the sign of $\Delta E_{\text{tot}}$ and $\Delta E_{\text{ext}}$ and consider only half of this last one following Eq. (21).

\[
\begin{align*}
\Delta E_{\text{tot}} &= \Delta E_{\text{cc}} + \Delta E_{\text{ext}} \quad \text{(20)} \\
\Delta E_{\text{tot}} &= -\Delta E_{\text{cc}} = 0.5 \cdot \Delta E_{\text{ext}}. \quad \text{(21)}
\end{align*}
\]

Figure 5 shows the two energy contributions to $\Delta E_{\text{tot}}$. The prediction of linear response is respected in the same range up to $V_0 \simeq 0.05 \text{ zJ}$. What we can extrapolate from the above is that the validity range of the NM theory in the numerical model is about $V_0 = 5 \cdot 10^{-4} \text{ zJ} : 0.05 \text{ zJ}$. Figure 5 shows that deviations from the linear-response regime at small $V_0$ are entirely due to the $\Delta E_{\text{ext}}$ term. The origin of these deviations are not entirely clear at the moment.

The first effect of non-linearity is associated to prevalence of $\Delta E_{\text{ext}}$ over $\Delta E_{\text{cc}}$. As $V_0$ increases beyond 0.4 zJ the colloid have come very close to the minima of the corrugation potential: from this point on, $\Delta E_{\text{cc}}$ increases only weakly and the total energy lowering is due mainly to $\Delta E_{\text{ext}}$. $|\Delta E_{\text{ext}}|$ will eventually keep increasing linearly in $V_0$. 
4.2 Comparison between theory and simulation

Within the linearity range we want to compare the dependence of the energy per colloid on the relative rotation of substrate and adsorbate as provided by the NM theory in Eq. (13) with that obtained from the relaxations. In all the comparisons examined we need to rescale the theory value by a factor 0.002, of unknown origin. Figures 6 and 7 show the difference between the theoretical and simulated angular dependence for a potential amplitude $V_0 = 0.01$ zJ (linearity range) and $V_0 = 0.1$ zJ (range of non-linearity). The first is in good agreement with the theoretical prediction, in particular with regard to the position of the Novaco angle, the minimum energy angle. The second instead shows a qualitatively different trend, with a completely different minimum energy angle.

To test the validity of the NM approach we repeat the simulations for other values of $a_{pot}$, in particular we explore the following values: 5.905, 6.2, 8.8, 9.554, 10.5 μm. They are reported in Fig. 8 and Fig. 9.

4.3 Dynamics

We introduce $F_{1s}$, namely the minimum force needed by a single colloid to exit the potential well at the origin. We will express the driving force in term of $F_{1s}$. In agreement with Ref. [11] the relation between $F_{1s}$, $a_{pot}$ and is $V_0$ given by:

$$F_{1s} = \frac{z V_0}{a_{pot}},$$

(22)
where \( z = 4.279396 \pm 0.000001 \).

Starting from the minimum energy configuration find in the linear range for \( a_{pot} = 5.2 \) \( \mu \)m, characterized by a relative angle \( \theta = 4^\circ \) (see Fig.6), we introduce an external force directed along the \( x \)-axis, which we increase ”adiabatically” in steps by \( 0.01 \cdot F_{1s} \). Two possible responses of the monolayer are observed, Fig. 10: either the monolayer move very little and stops at the slight displace equilibrium position (static pinning), or the monolayer keeps advancing in reaction to the force (unpinned sliding state).

We examine this frictional dynamics for several values of corrugation amplitude \( V_0 \). Figure 11 shows the mobility \( \langle v_{cm} \rangle /F \) of the monolayer as a function of the driving force, starting from the same kind of fully relaxed configuration at \( \theta = 4^\circ \). For strong corrugation , \( V_0 = 1 \) zJ, a clear pinned-unpinned transition is observed at a static friction force \( F_s = 0.25 F_{1s} \). A similar behavior also occurs for smaller corrugation amplitude, 0.25 and 0.5 zJ. For \( V_0 < 0.1 \) zJ we find superlubrics sliding state, namely a state in which even very small external forces induce a translation. Of course for smaller potential amplitude, in particular those in the linear range, we expect the same condition. As usual in this context a finite-size simulation cannot assess a perfect superlubric state due to a weak residual pinning associated to the boundary particles. This observation could explain the drop mobility at extremely small \( F/F_{1s} \). The existence of a static-friction state in unclear for \( V_0 = 0.1 \) zJ.

To speed up the simulations we find that the FIRE algorithm is quite advantageous compared to the standard MD for the first part of the frictional simulations, namely in the static regime. As soon as the unpinned state is reached,
Figure 8: Same as Fig.6 but with $a_{pot} = 5.905 \mu m$ and 6.2 µm. $V_0 = 0.01 \ zJ$.

Figure 9: Same as figure 6 but with $a_{pot} = 8.8 \mu m$, 9.554 µm and 10.5 µm. $V_0 = 0.01 \ zJ$. 
the absence of an energy minimum is clearly signaled by the FIRE minimization not converging and rather keeping accelerating. Once we locate the minimum force value that corresponds to an unpinned state we restart the force stepwise increase using the standard MD integration from the previous pinned state.

We conclude that at the Novaco angle all the linear range up to $V_0 = 0.01 \text{ zJ}$ is characterized by superlubric sliding. In the range $V_0 = 0.25 - 1 \text{ zJ}$ instead we demonstrate a pinned-unpinned transition characterized by a static friction $F_s/F_{1s}$ ranging approximately from 0.2 to 0.25. According to our simulations the Aubry transition between the zero-static friction superlubric state and finite static friction occurs near $V_0 = 0.1 \text{ zJ}$.

### 5 Discussion and Conclusion

The main conclusion that we have reached are the following:

- The validity range of the Novaco theory is approximately $V_0 = 5 \cdot 10^{-4} - 0.05 \text{ zJ}$. The lower boundary seems to be due to residual forces associated to the numerical precision of computers. The upper boundary marks the onset of non-linear effect due to the strongly non-linear nature of the Yukawa inter-particle interaction.
Figure 11: Pinned-unpinned transition for $V_0 = 1, 0.5, 0.25$ and $0.01$ zJ. $a_{\text{pot}} = 5.2 \mu m$, $a_{\text{coll}} = 5.8 \mu m$.

- In this linear range the comparison between theoretical and minimized energy lowering as a function of the misalignment angle between substrate and adsorbate are in good agreement, except for a 0.002 factor of unknown origin. Outside this range the angle-energy relation changes substantially. In particular the minimum-energy angle can deviate significantly from the Novaco angle.

- All the linear range where the NM theory holds is characterized by a superlubric sliding. The corrugation $V_0 = 0.1$ zJ marks the Aubry boundary between a pinned region with a clear static friction threshold and a superlubric sliding region at a weaker corrugation.

Several aspects of this research deserve further consideration:

- We need to clarify the origin of the proportionality factor between theoretical and minimization energy from the computed model.

- It may be convenient to adopted a hexagonal Wigner-Seitz supercell to reduce boundary effects in the minimization of the energy-angle dependence.

- It is worth to investigate odd-$N$ supercell which have one particle at their center of mass rather than the center of triangle. This change may make a difference for the energy lowering associated to global translation.
• Friction should certainly be investigated for other values of the mismatch ratio $a_{pot}/a_{coll}$.
References


