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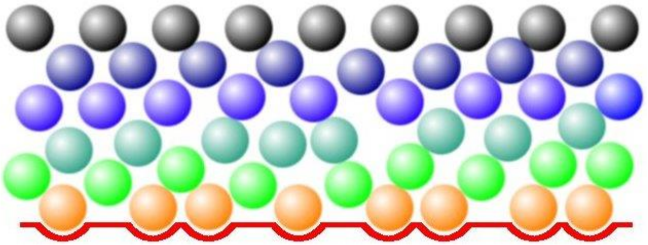


Michael Schmiedeberg

Growth of Soft Quasicrystals

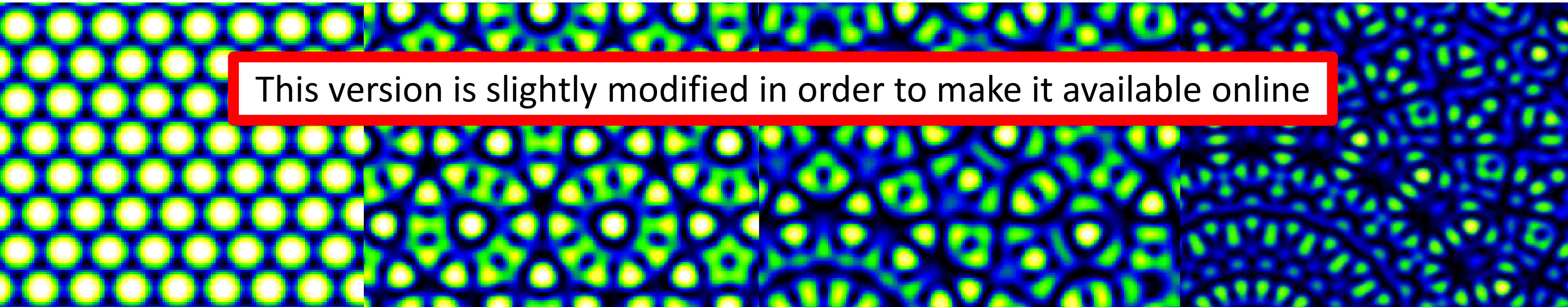
in cooperation with:

M. Martinsons, A. Gemeinhardt, B. Decker, K. Lenk,

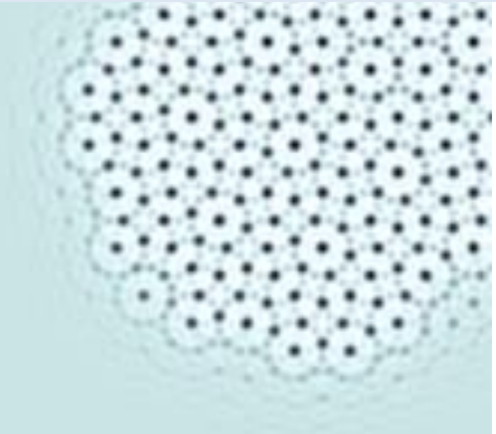
J. Hielscher, S.C. Kapfer (FAU Erlangen),

C.V. Achim (Conceptión, Chile), E.C. Oguz (Tel Aviv),

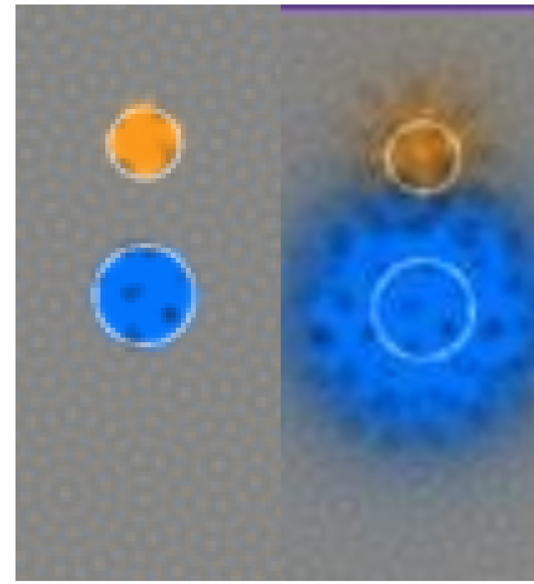
Matthias Sandbrink, Hartmut Löwen (HHU Düsseldorf)



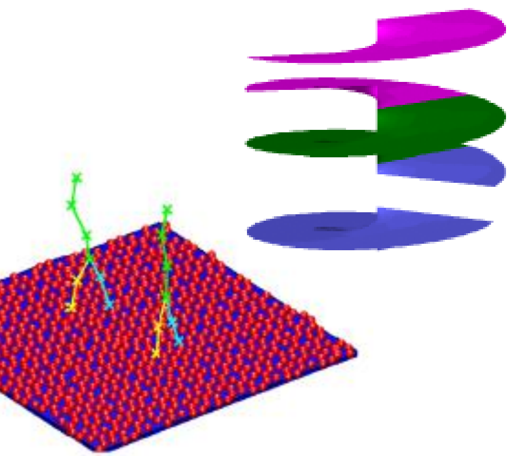
Outline



Dynamical PFC model
predicts different growth modes
due to phasons

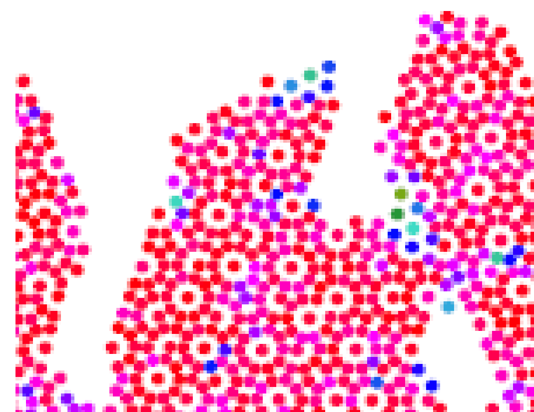


Growth from two seeds:
Less dislocations due to phasons



Side notes:
Dislocation lines and
screw dislocations in 3D

Simulations of the growth in 2D:
Isotropic interactions
vs. preferred binding angles



Phase Field Crystal Model (PFC)

Expansion of the free energy with respect to an order parameter $\psi(\vec{x})$:

For periodic crystals (one length scale):

$$F = \int d\vec{x} \left[\frac{\psi}{2} \left(r + \left(k_0^2 + \nabla^2\right)^2 \right) \psi + \frac{\psi^4}{4} \right]$$

For quasicystals two length scales:

$$\left(k_1^2 + \nabla^2\right)^2 \left(k_2^2 + \nabla^2\right)^2$$

Length scales:

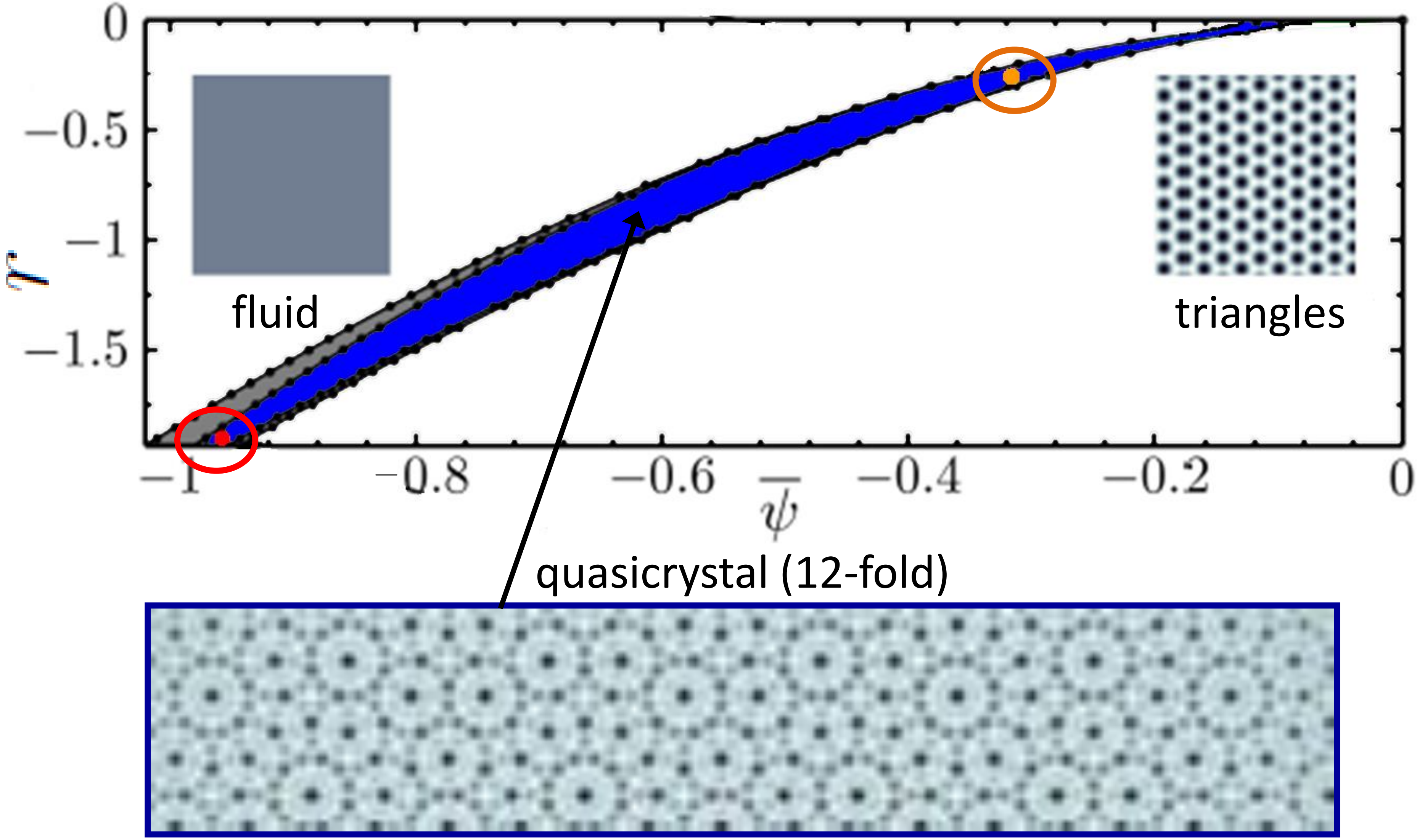
$$k_2^2 / k_1^2 = \left[1 - \cos(2\pi/N)\right] / \left[1 - \cos(4\pi/N)\right] \qquad N = 5, 8, 10, 12$$

Dynamics: $$\frac{\partial \psi}{\partial t} = \nabla^2 \frac{\delta F[\psi]}{\delta \psi}$$

Parameters: r (temperature) $\bar{\psi}$ (mean density)

C.V. Achim, M.S., H. Löwen, PRL **112**, 255501 (2014)
cf. J. Rottler, M. Greenwood, B. Ziebarth, J. Phys.: Condens. Matter **24**, 135002 (2012)
Faraday waves: R. Lifshitz, D.M. Petrich, Phys. Rev. Lett. **79**, 1261 (1979)

PFC-phase diagram (2D)



C.V. Achim, M.S., H. Löwen, PRL **112**, 255501 (2014).

Growth of decagonal quasicrystals

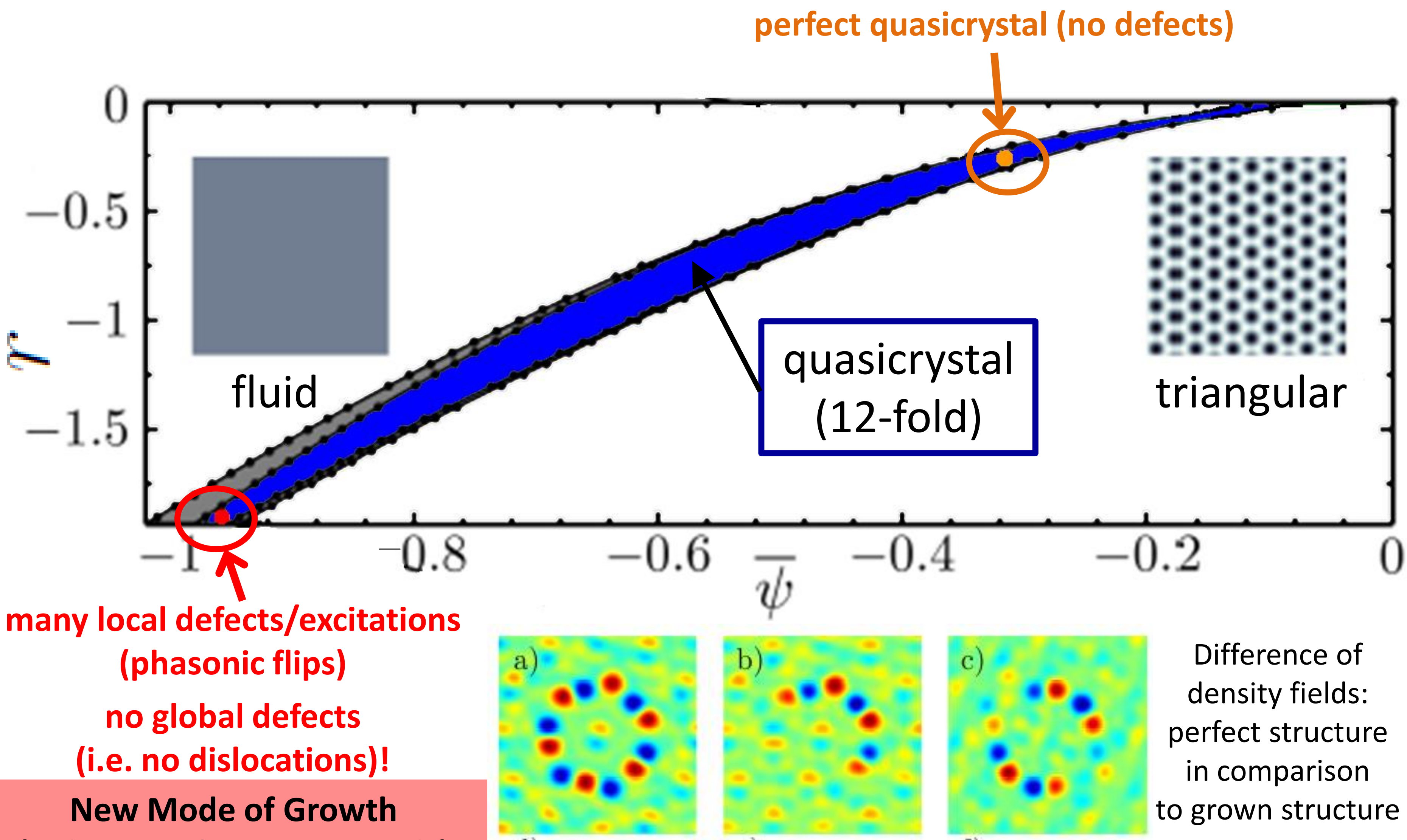
Growth with many phasonic flips:

Perfect growth:

The movies are available as supplemental materials of
C.V. Achim, M.S., H. Löwen, PRL **112**, 255501 (2014).
see:
https://journals.aps.org/prl/supplemental/10.1103/PhysRevLett.112.255501
movie-fig2b.avi and movie-fig2e.avi

C.V. Achim, M.S., H. Löwen, PRL **112**, 255501 (2014).

Two different Growth Modes



many local defects/excitations
(phasonic flips)

no global defects
(i.e. no dislocations)!

New Mode of Growth
(only exists for quasicrystals)

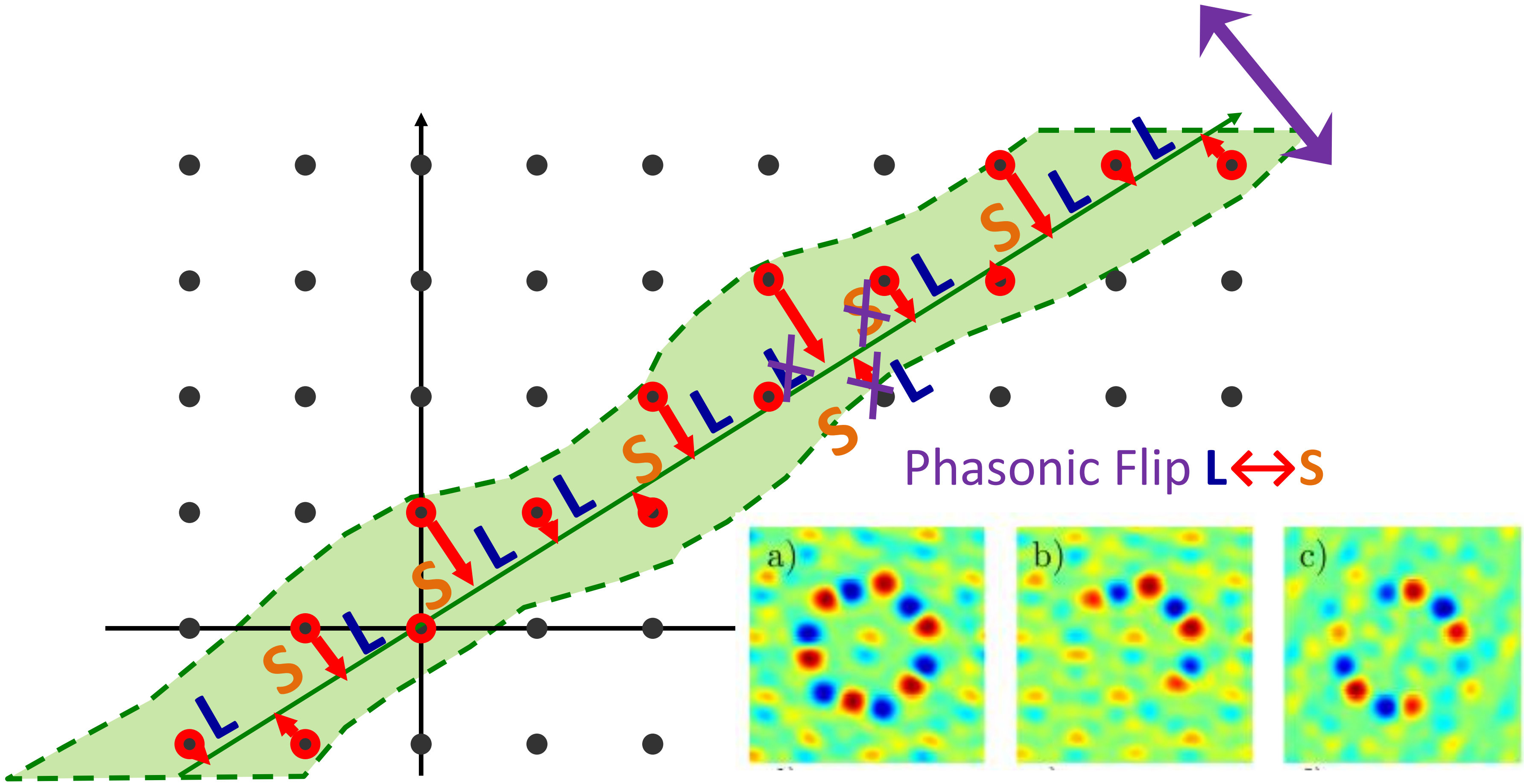
Difference of density fields: perfect structure in comparison to grown structure

C.V. Achim, M.S., H. Löwen, PRL **112**, 255501 (2014).

Additional degrees of freedom

Displacement parallel to the physical space: Phonon

Displacement perpendicular to the physical space: Phason



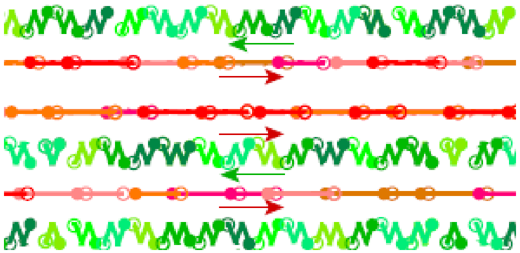
Additional degrees of freedom: Phasons

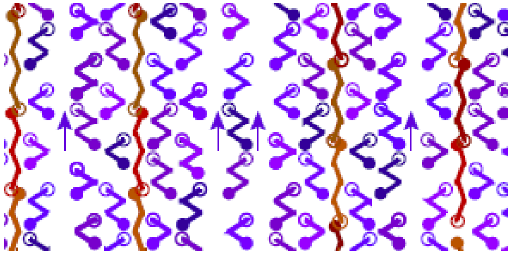
Phason in x-direction

Phason in y-dirction

Similar movies are available as supplemental materials of
J.A. Kromer, M. S., J. Roth, and H. Stark, Phys. Rev. Lett. **108**, 218301 (2012).
see:
https://journals.aps.org/prl/supplemental/10.1103/PhysRevLett.108.218301
collective_motion_x-phason.avi and collective_motion_y-phason.avi

straight path
in +x -direction
or: zig-zag-path
in -x -direction

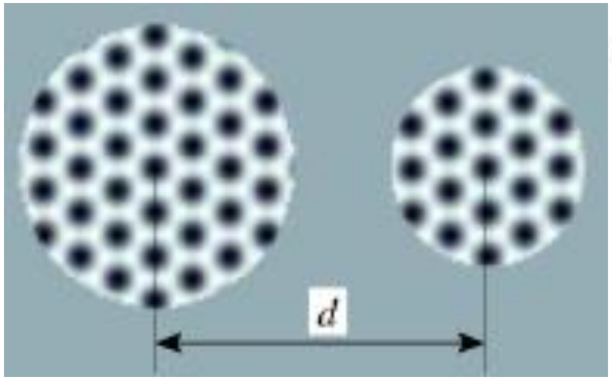


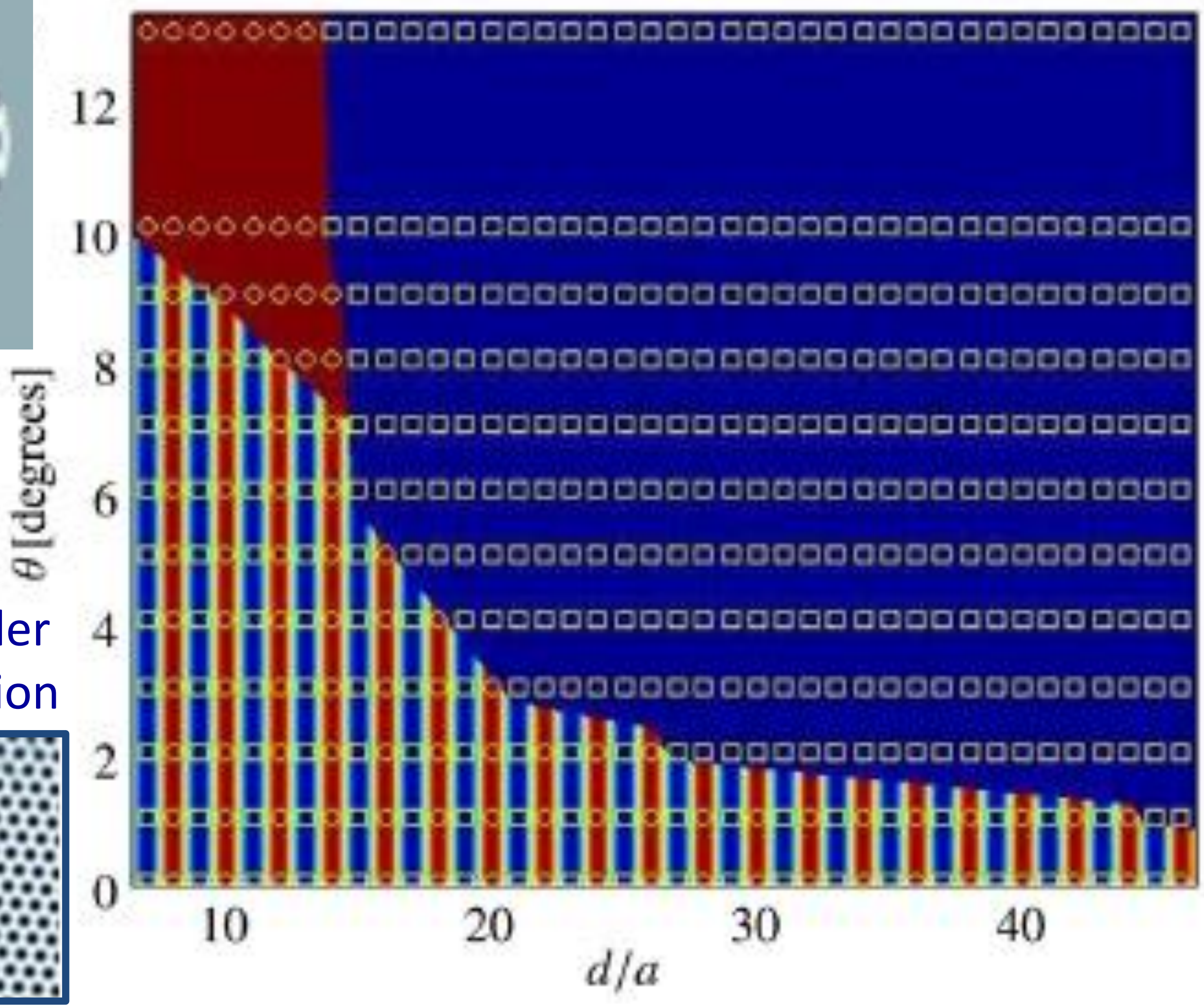


zig-zag-path
in +y -direction
or: zig-zag-path
in -y -direction

J.A. Kromer, M. S., J. Roth, and H. Stark, Phys. Rev. Lett. **108**, 218301 (2012)

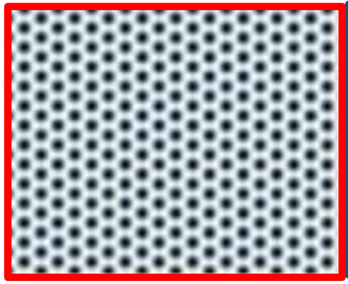
Growth from two seeds: Periodic Crystal

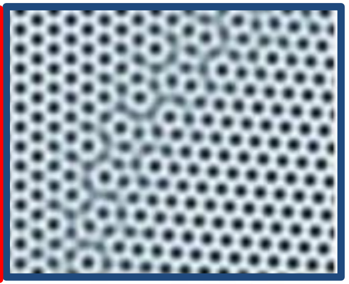




red:
no
dislocations

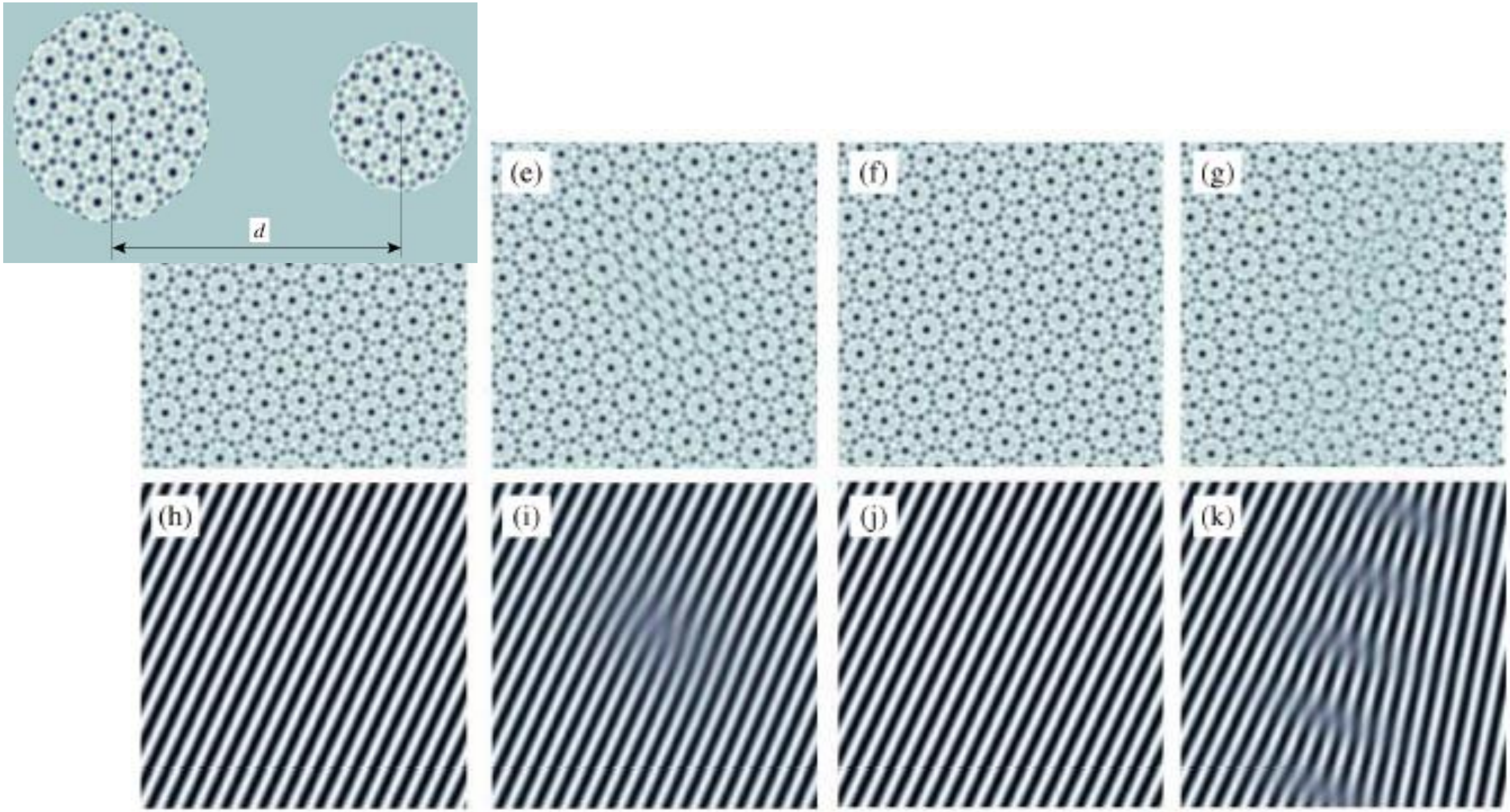
blue:
domain border
with dislocation





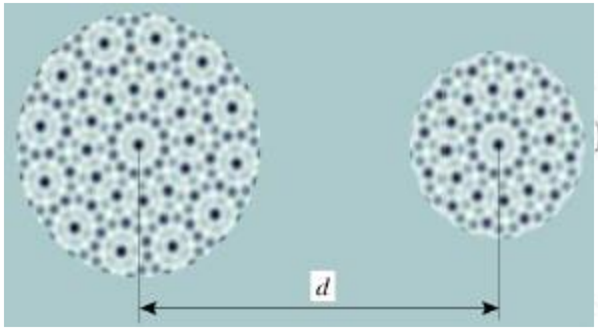
M. S., C.V. Achim, J. Hielscher, S. Kapfer, and H. Löwen, Phys. Rev. E **96**, 012602 (2017).

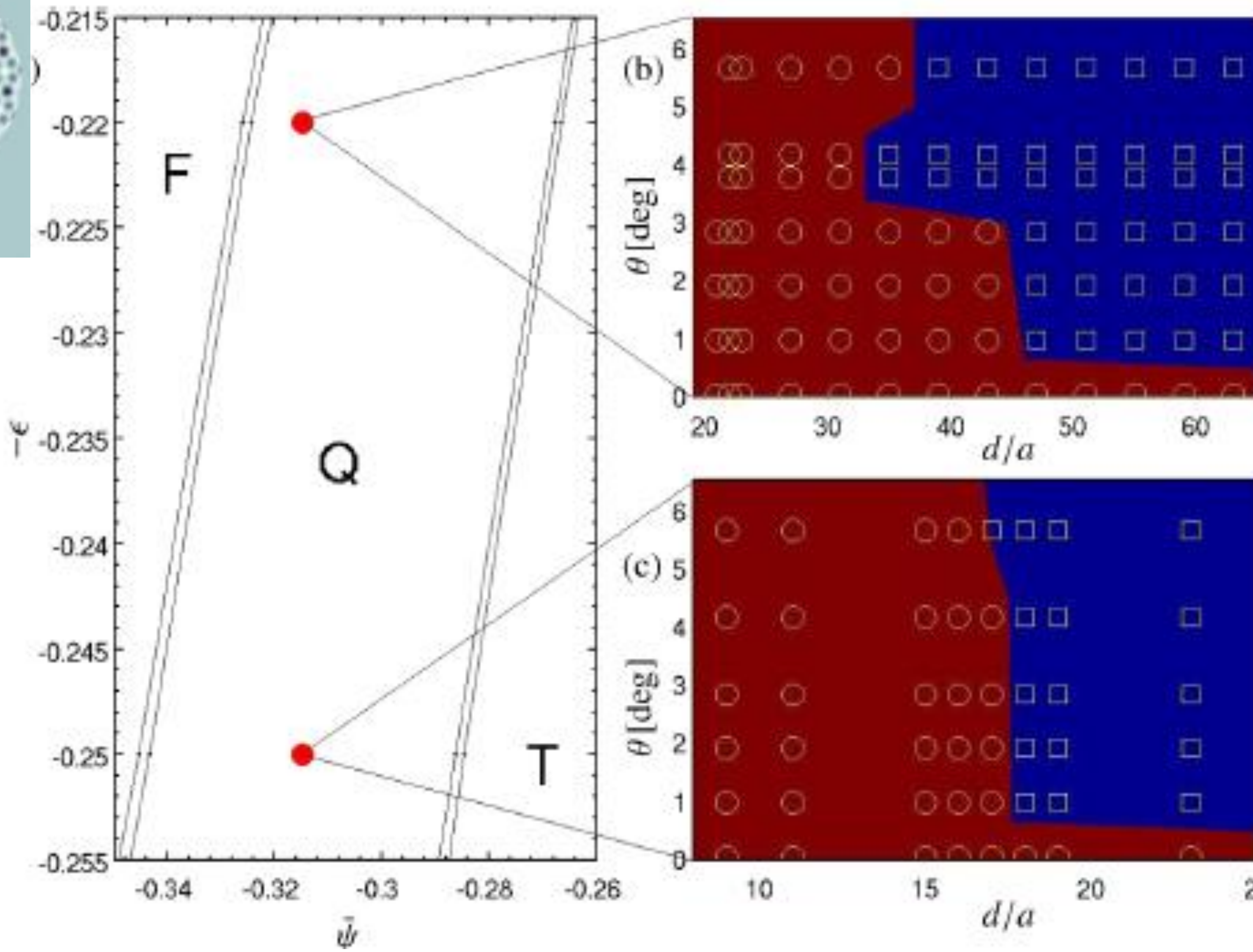
Growth from two seeds: Quasicrystal



M. S., C.V. Achim, J. Hielscher, S. Kapfer, and H. Löwen, Phys. Rev. E **96**, 012602 (2017).

Growth from two seeds: Quasicrystal



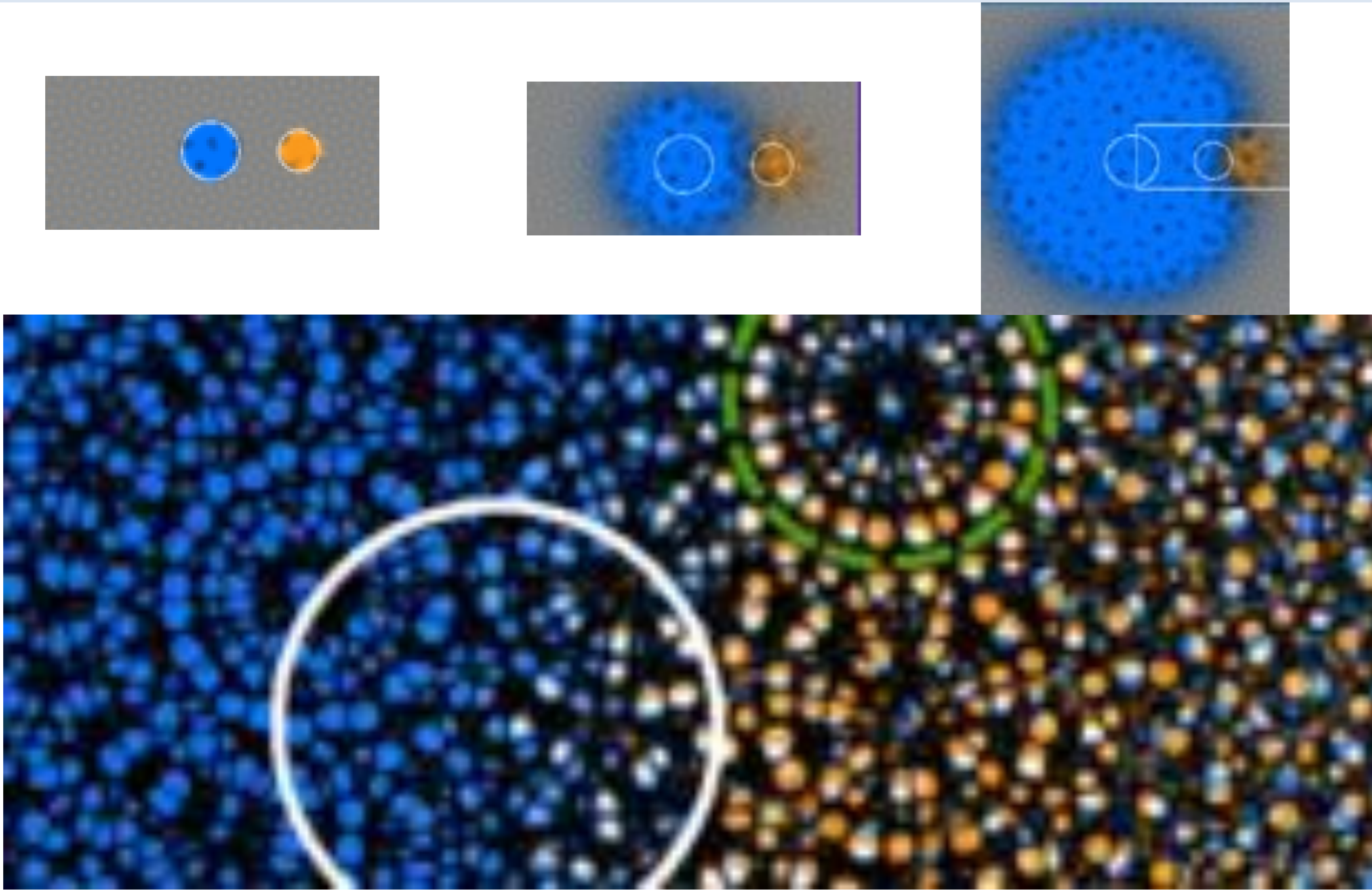


red:
no
dislocations

blue:
domain border
with dislocation

M. S., C.V. Achim, J. Hielscher, S. Kapfer, and H. Löwen, Phys. Rev. E **96**, 012602 (2017).

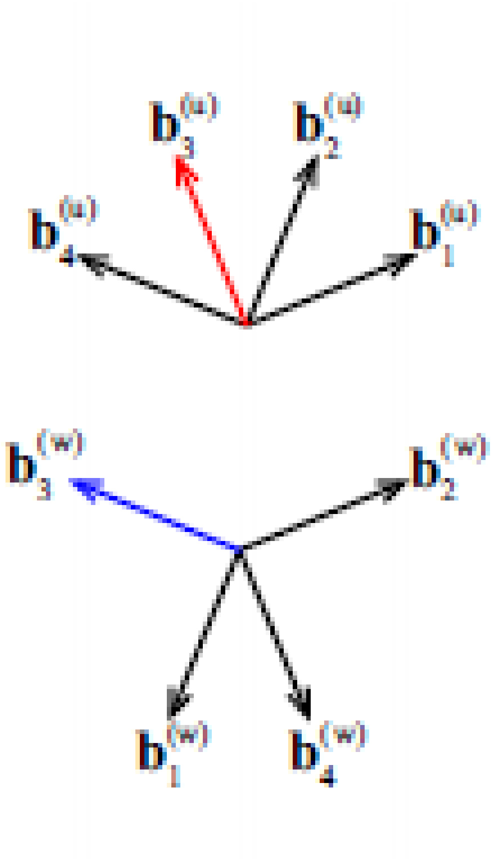
Quasicrystal: Incorporation by phasonic flips

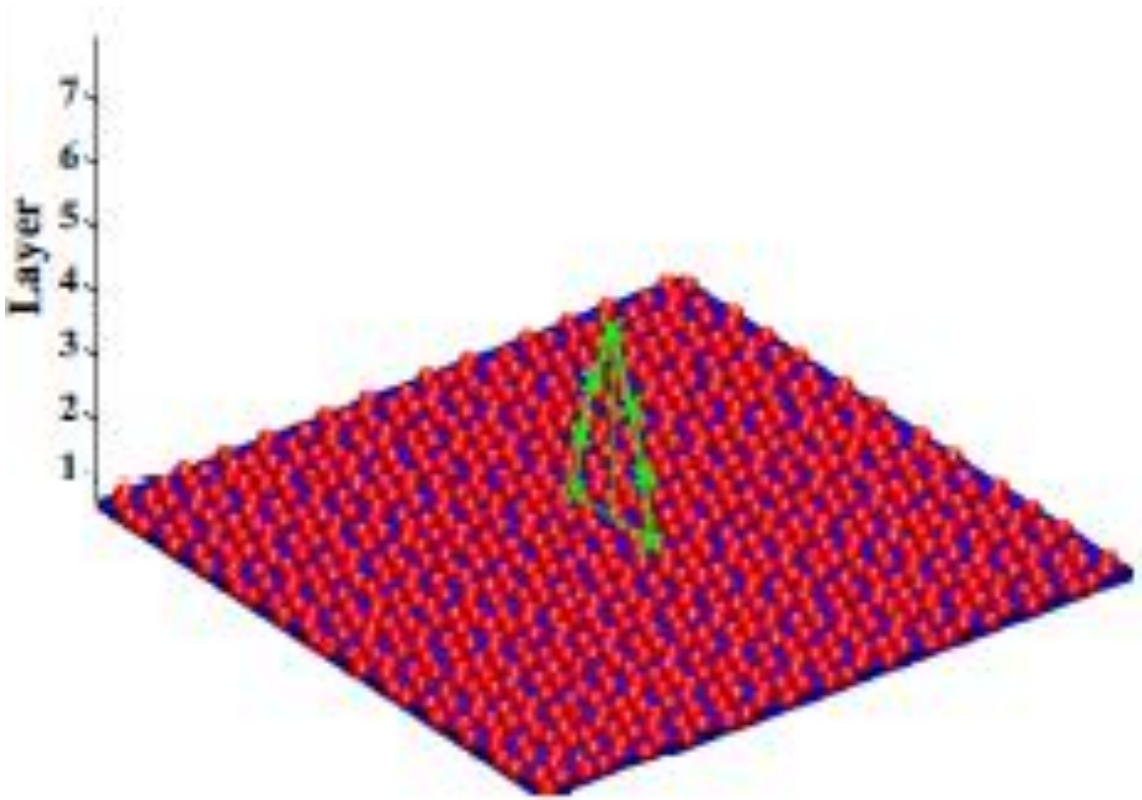


M. S., C.V. Achim, J. Hielscher, S. Kapfer, and H. Löwen, Phys. Rev. E **96**, 012602 (2017).

Side Note: Dislocation lines in 3D

Annihilation

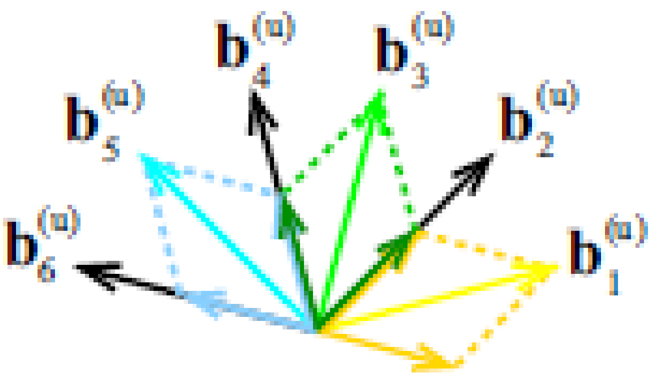


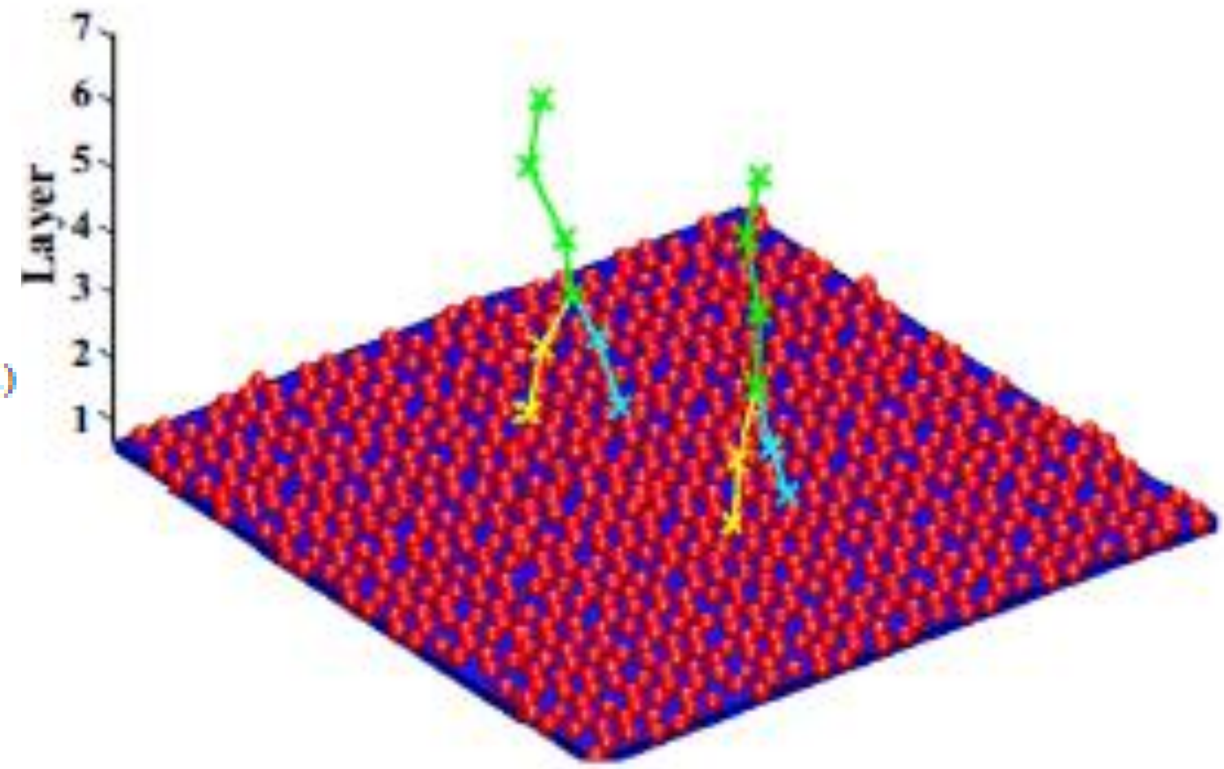


M. Sandbrink and M. S., Phys. Rev. B **90**, 064108 (2014).

Side Note: Dislocation lines in 3D

Partial Annihilation

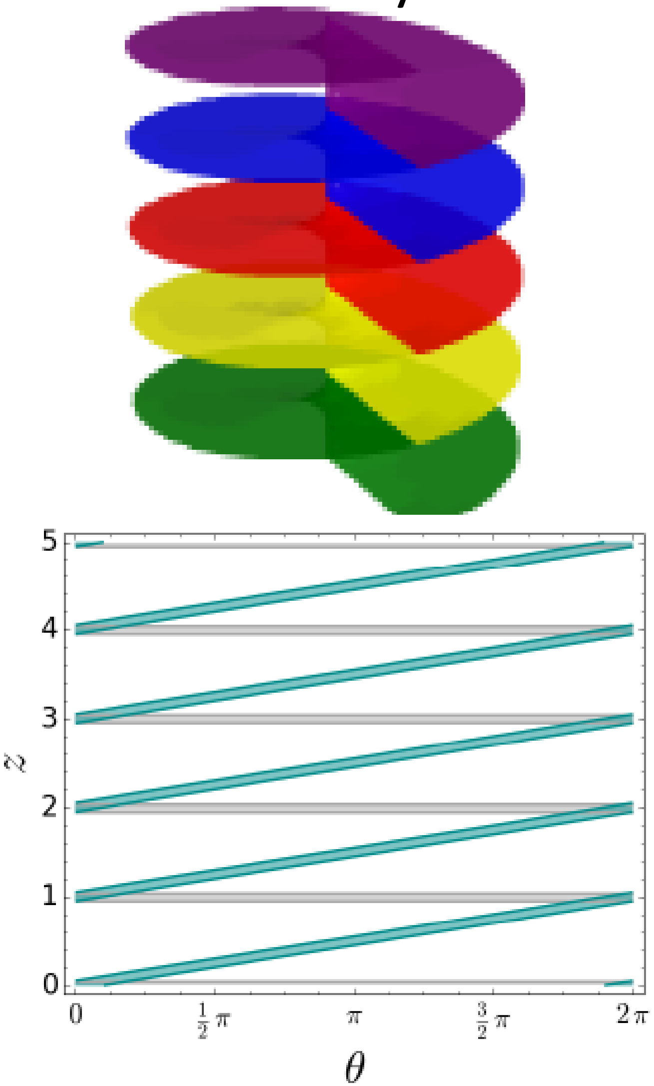




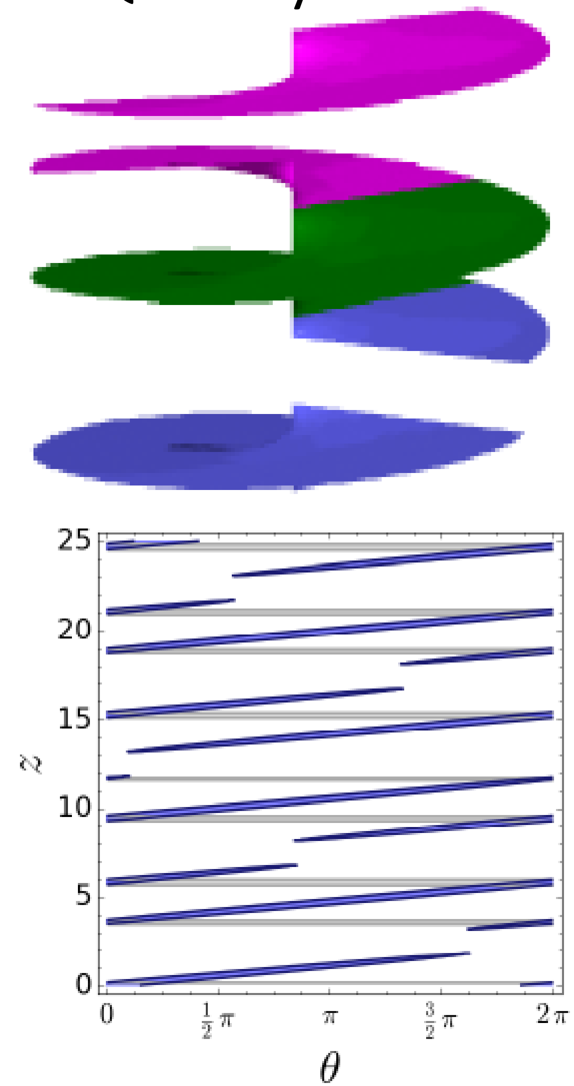
M. Sandbrink and M. S., Phys. Rev. B **90**, 064108 (2014).

Side Note: Screw Dislocations

Periodic Crystals



Quasicrystals



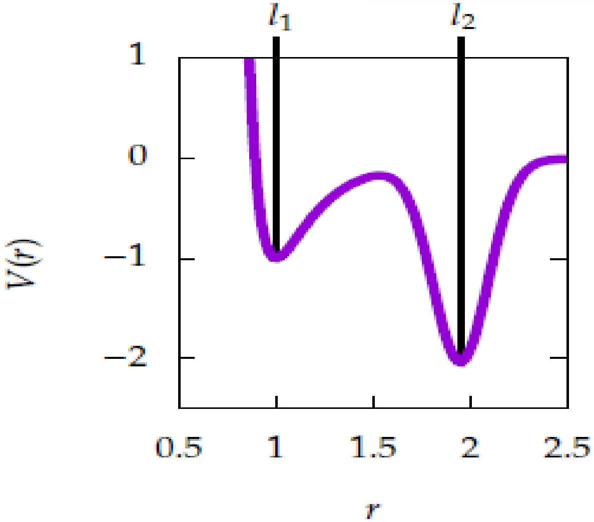
Calculations and figures by K. Lenk.

Simulations in 2D: Isotropic vs. patchy colloids

Brownian dynamics simulations

isotropic
Lennard-Jones-Gauss potential

$$V_{LJG}(r) = \frac{1}{r^{12}} - \frac{2}{r^6} - \epsilon \exp\left(-\frac{(r-r_G)^2}{2\sigma^2}\right)$$

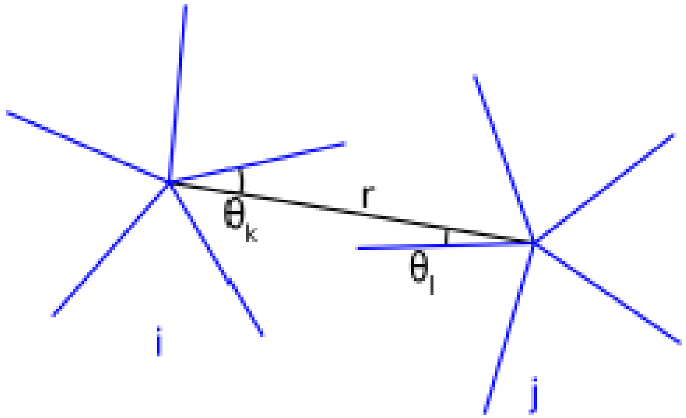


here:
10-fold
or
12-fold

cf. Engel, Trebin,
PRL **98**, 225505 (2007).

patchy colloids
with preferred binding angles

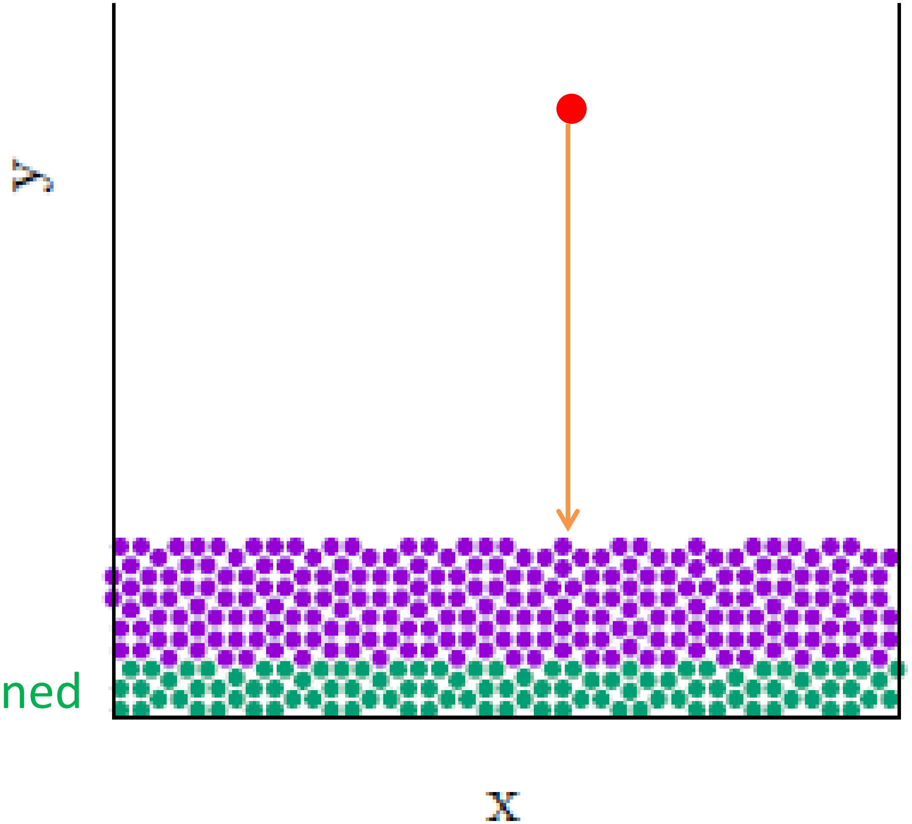
$$V(r.\theta_k,\theta_l) = \left(\frac{1}{r^{12}} - \frac{2}{r^6}\right) \cdot \exp\left(-\frac{\theta_k^2}{2\sigma_{pw}^2}\right) \exp\left(-\frac{\theta_l^2}{2\sigma_{pw}^2}\right)$$



here:
12-fold

cf. van der Linden et al.,
J. Chem. Phys. **136**, 054904 (2012).

Simulations in 2D: Setup



new particles
are inserted
with a rate R
at random x-position
and forced downwards
onto the surface

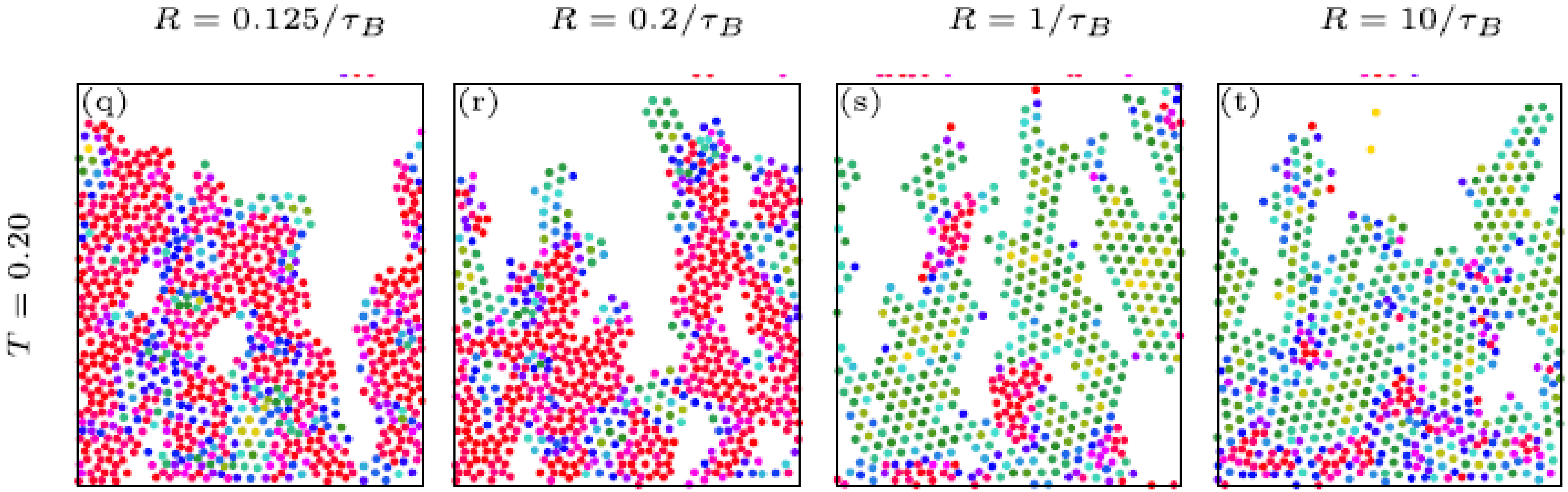
Substrate:
initially perfect
quasicrystal
green colloids are pinned

Simulations by M. Martinsons (isotropic) and A. Gemeinhardt (patchy).

Decagonal with isotropic interactions

Low temperature:

triangles at large rates

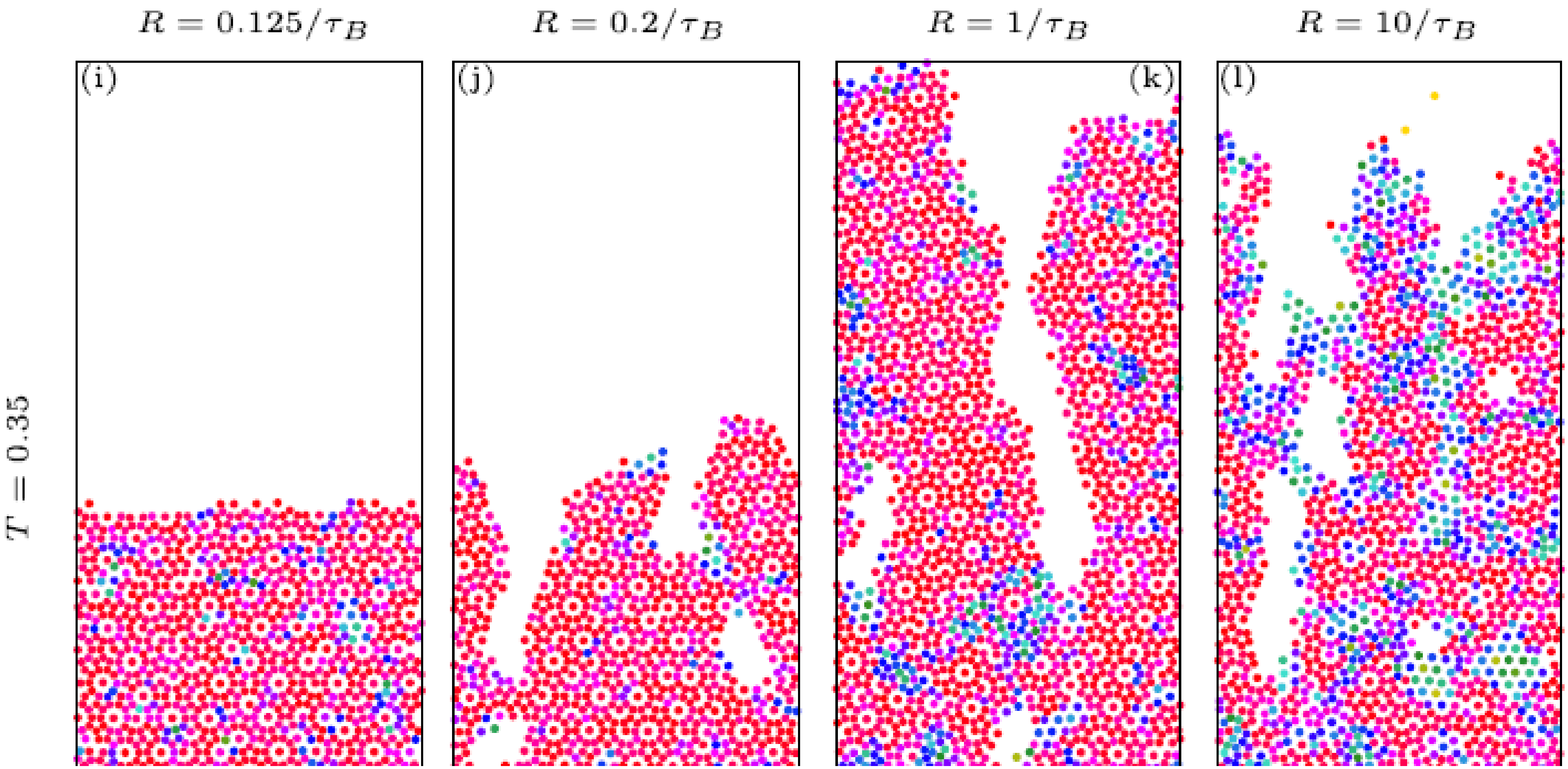


M. Martinsons and M. S., J. Phys.: Condens. Matter 30,255403 (2018).

Decagonal with isotropic interactions

Intermediate temperatures:

Faceted surfaces, especially at larger rates

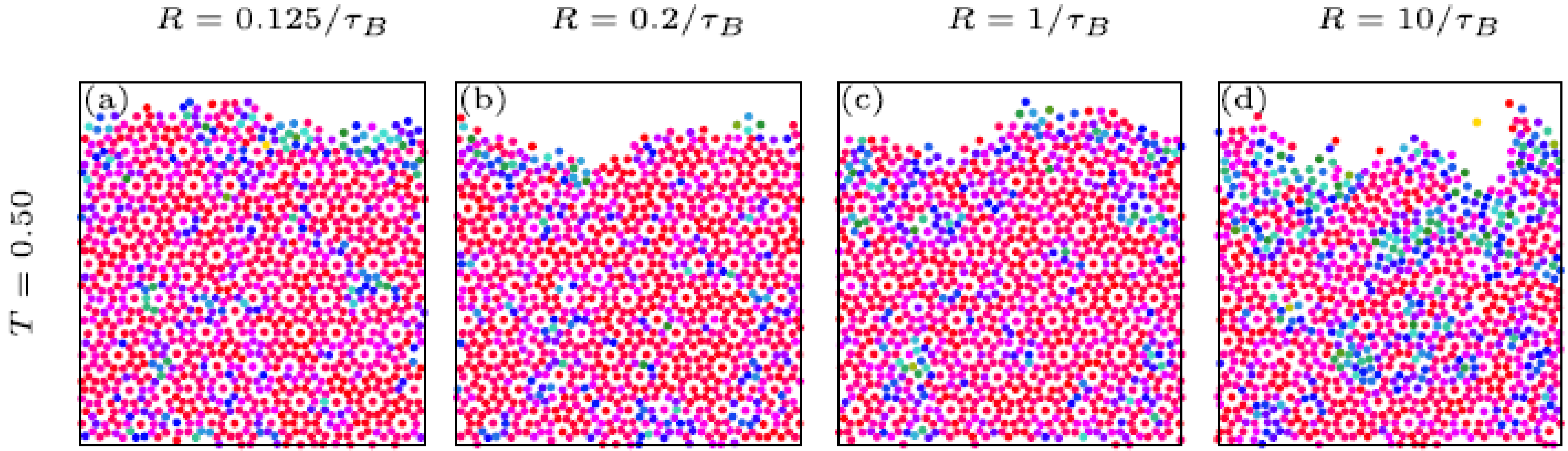


M. Martinsons and M. S., J. Phys.: Condens. Mattter 30,255403 (2018).

Decagonal with isotropic interactions

Large temperatures:

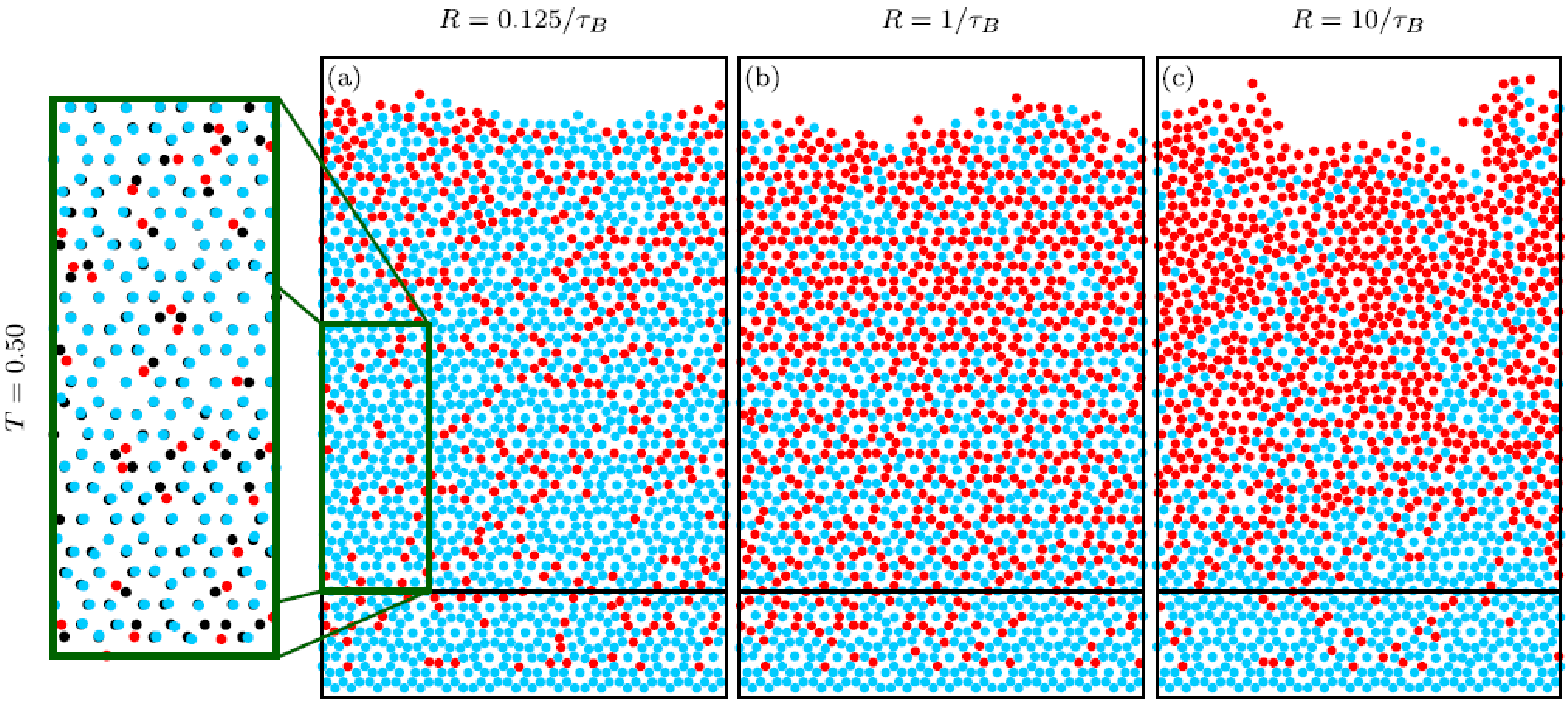
Nice quasicrystals, especially at low rates



M. Martinsons and M. S., J. Phys.: Condens. Mattter 30,255403 (2018).

Decagonal with isotropic interactions

Phasonic flips:

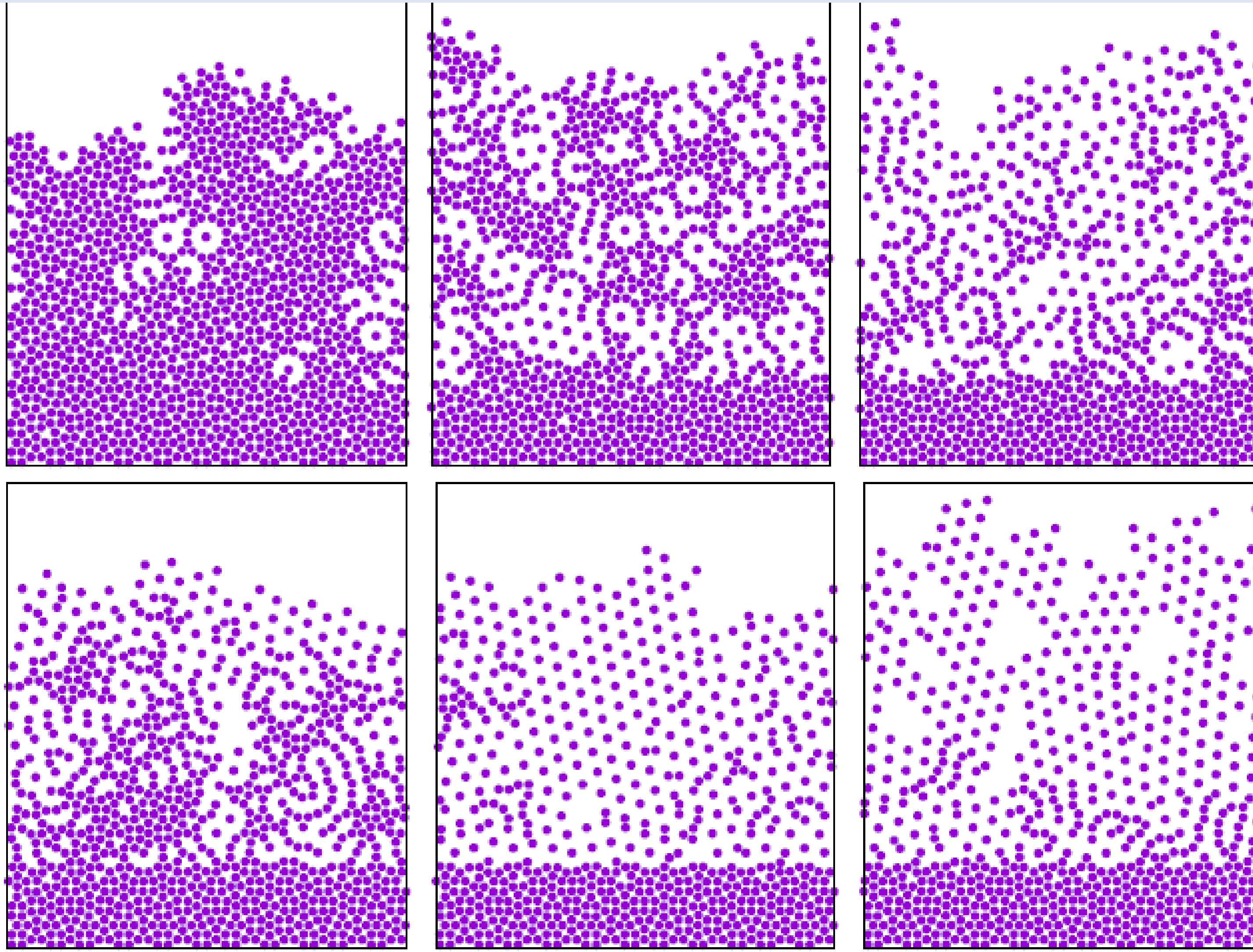


M. Martinsons and M. S., J. Phys.: Condens. Mattter 30,255403 (2018).

Dodecagonal with Isotropic interactions

T=0.04

T=0.02

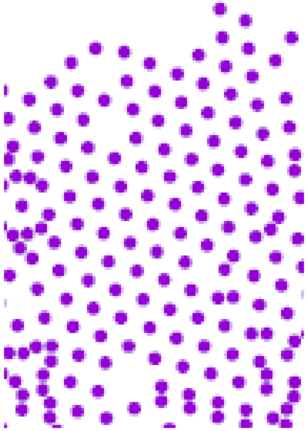


(a) $R = 0.125/\tau_B$ (b) $R = 0.5/\tau_B$ (c) $R = 10/\tau_B$

Simulations by M. Martinsons (isotropic) and A. Gemeinhardt (patchy).

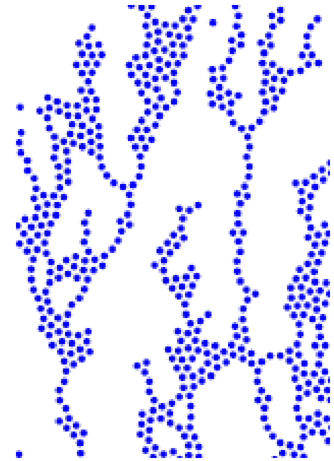
Dodecagonal: Isotropic vs. Patchy

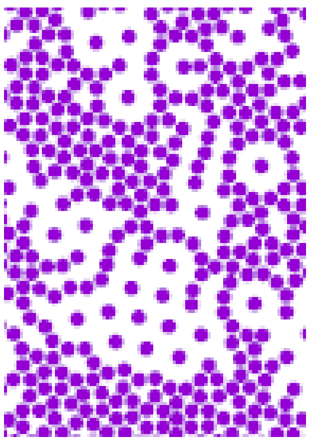
Isotropic: **Patchy:**



Triangles at low T

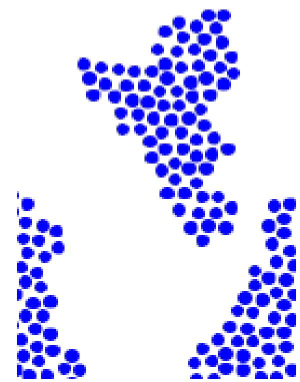
Gel-like structures at low T

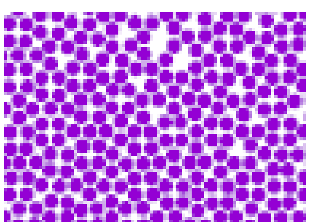




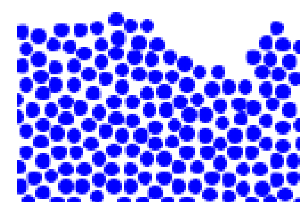
Excess of wheel structures

Deattached clusters at large rates





Best quasicrystals at large T and low rates



Simulations by M. Martinsons (isotropic) and A. Gemeinhardt (patchy).

Open question

10-fold vs. 12-fold

monodisperse system with isotropic interactions

seem to prefer 12-fold structures

Explanation by Ron Lifshitz:
More triangles in 12-fold structure,
triangles stabilize a structure

monodisperse system with preferred binding angles

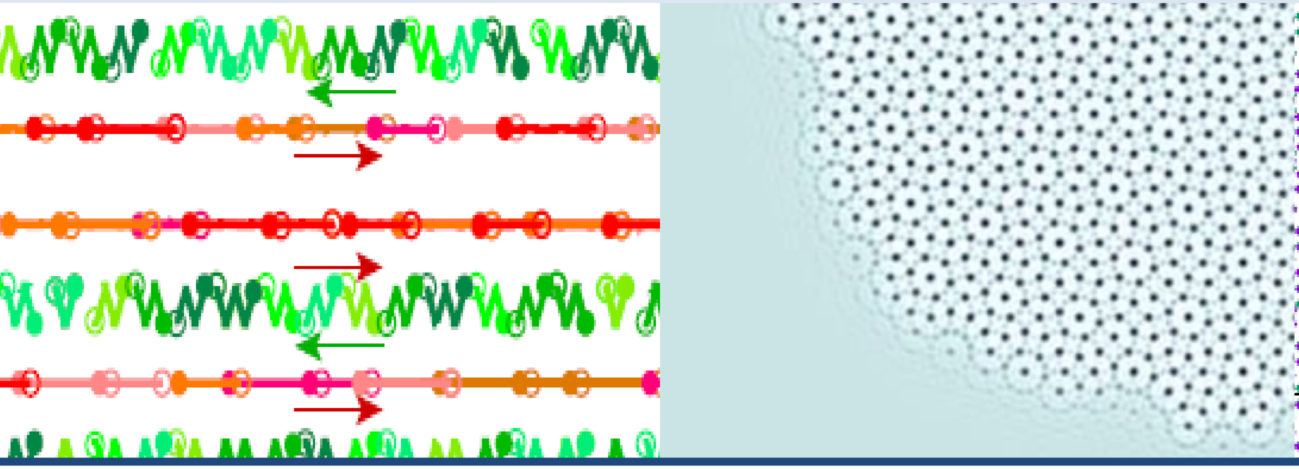
12-fold structures has been observed
10-fold possible

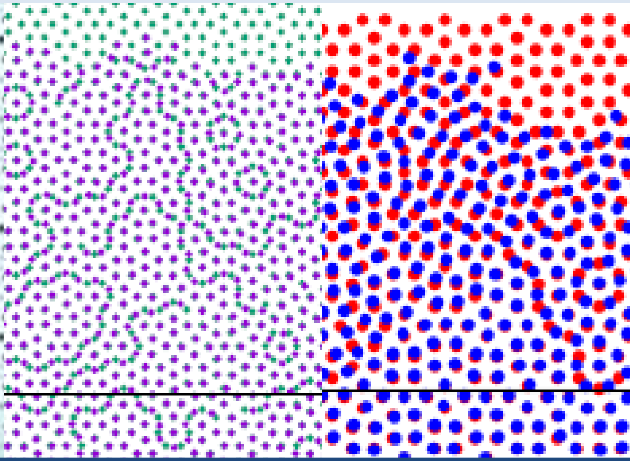
What systems prefer 10-fold ordering?

Are preferred binding angles enough for such a preference?

Multi-component systems necessary?

Conclusions





Special growth properties due to the additional degrees of freedom in quasicrystals

Isotropic vs. patchy

Acknowledgement

Group: M. Martinsons, A. Gemeinhardt, M. Sandbrink, B. Decker, K. Lenk
Erlangen: J. Hielscher, S.C. Kapfer, **Tel Aviv:** E.C. Oguz, **Bio-Bio:** C.V. Achim, **Stuttgart:** J. Roth
Düsseldorf: H. Löwen, **Berlin:** H. Stark, F. Rühle, J. Kromer, **Konstanz:** C. Bechinger
Financial support: *DFG (Emmy Noether Program), SFF (HHU Düsseldorf)*

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michael.schmiedeberg@fau.de