

SFB 951 HIOS

Project A7 (Klapp/Dzubiella)

(merged from A1 and A7)

# Project development 1<sup>st</sup> funding period

## A1 (Dzubiella):

Exploring HIOS structure formation by all-atom Molecular Dynamics (MD) simulations

## A7 (Klapp):

Coarse-grained simulations (MD, Monte-Carlo, kinetic MC) for growth phenomena and phase transitions of HIOS

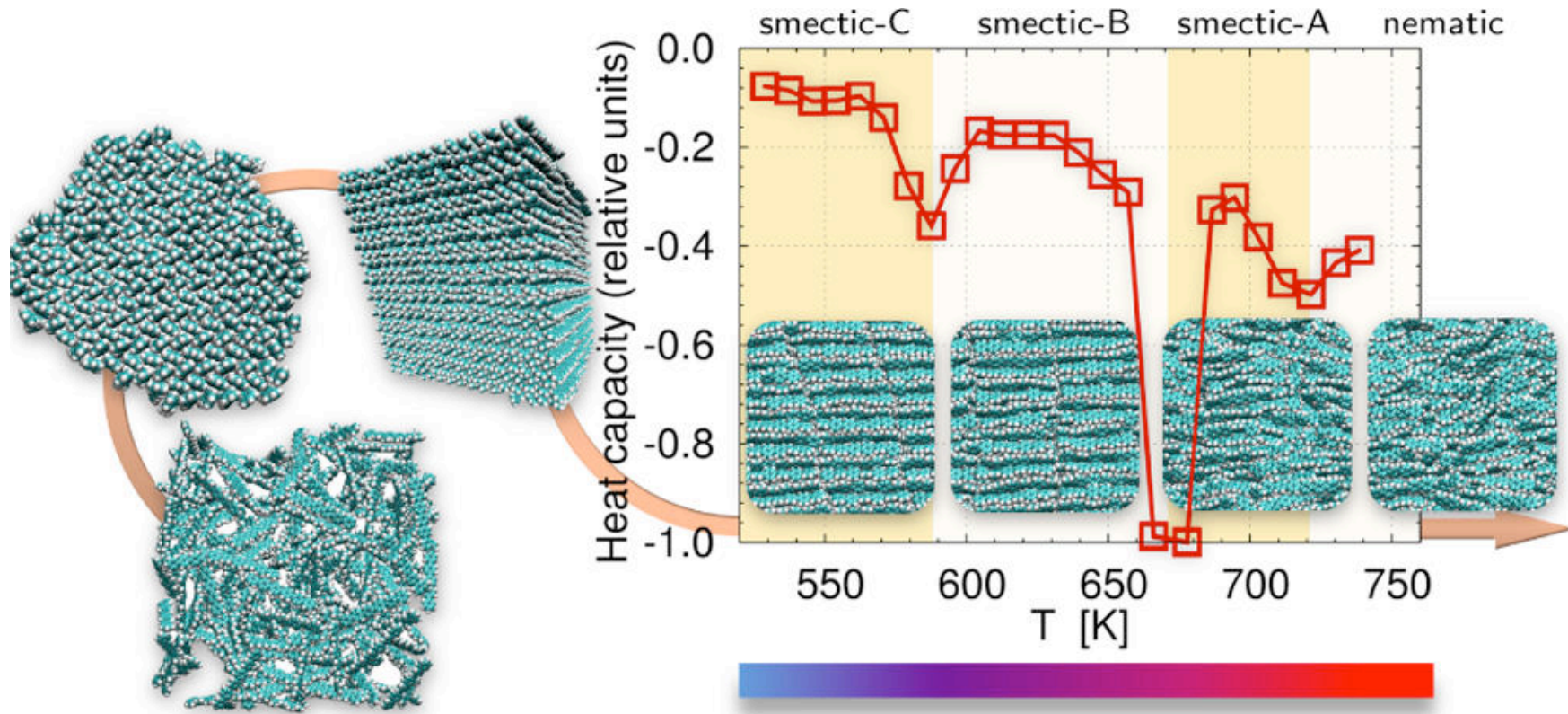
## Joint work A1/A7:

Systematic derivation of coarse-grained interaction potentials

# A1 (Dzubiella): Achievements 1st period

Growth of realistic bulk crystals of polyphenylens 'from scratch':  
Full characterization of structure and phase behavior

with A4

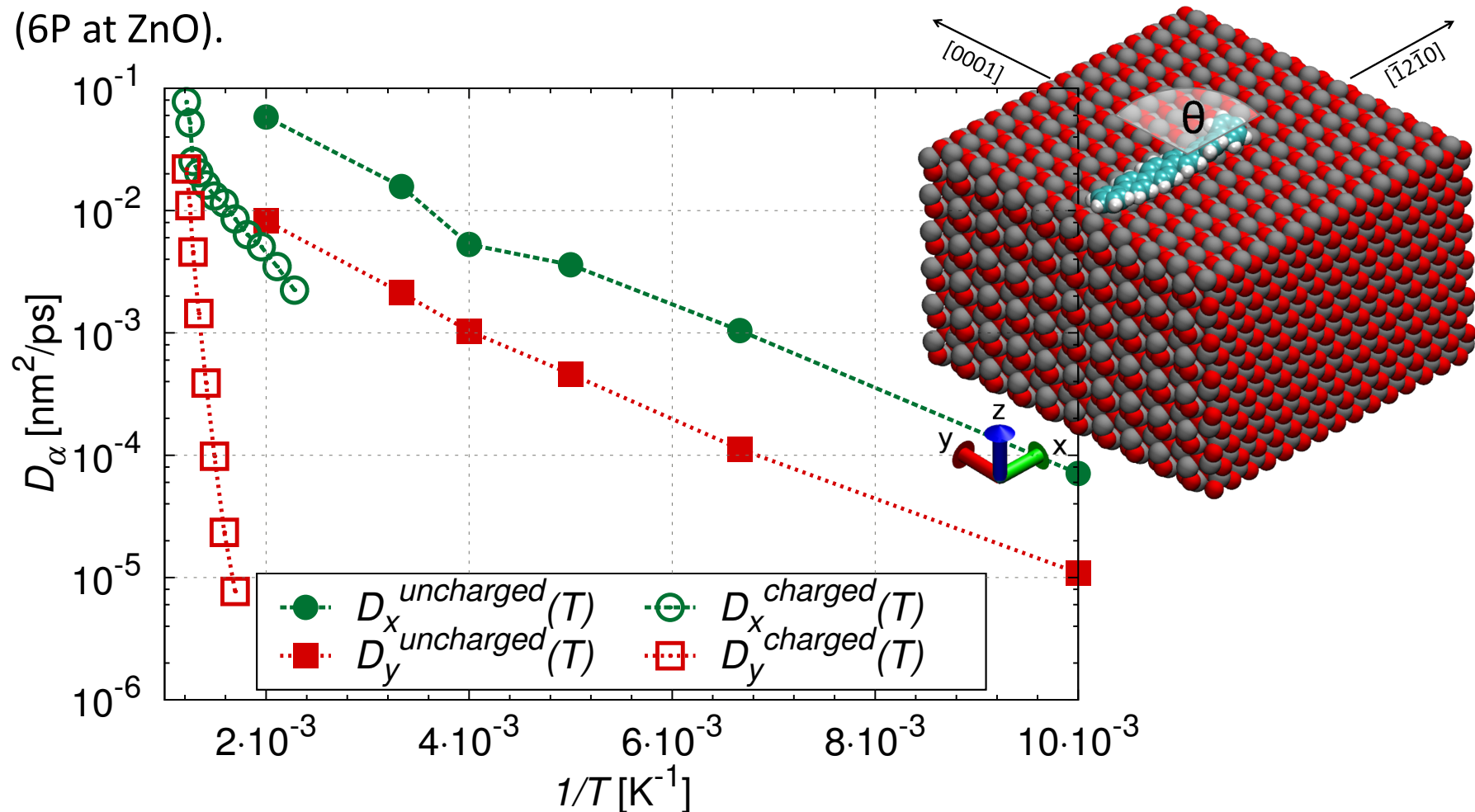


[Growth and characterization of molecular crystals of \*para\*-sexiphenyl by all-atom computer simulations](#)

K. Palczynski, G. Heimel, J. Heyda, and J. Dzubiella, *Crystal Growth and Design* **14**, 3791 (2014).

# A1 (Dzubiella): Achievements 1st period

Strongly anisotropic diffusion and transport due to electrostatic surface pattern (6P at ZnO).

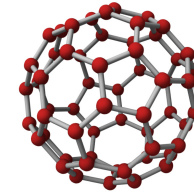


## Anisotropic electrostatic friction of para-sexiphenyl on ZnO surfaces

K. Palczynski and J. Dzubiella, *J. Phys. Chem. C*, first revision resubmitted (2014)

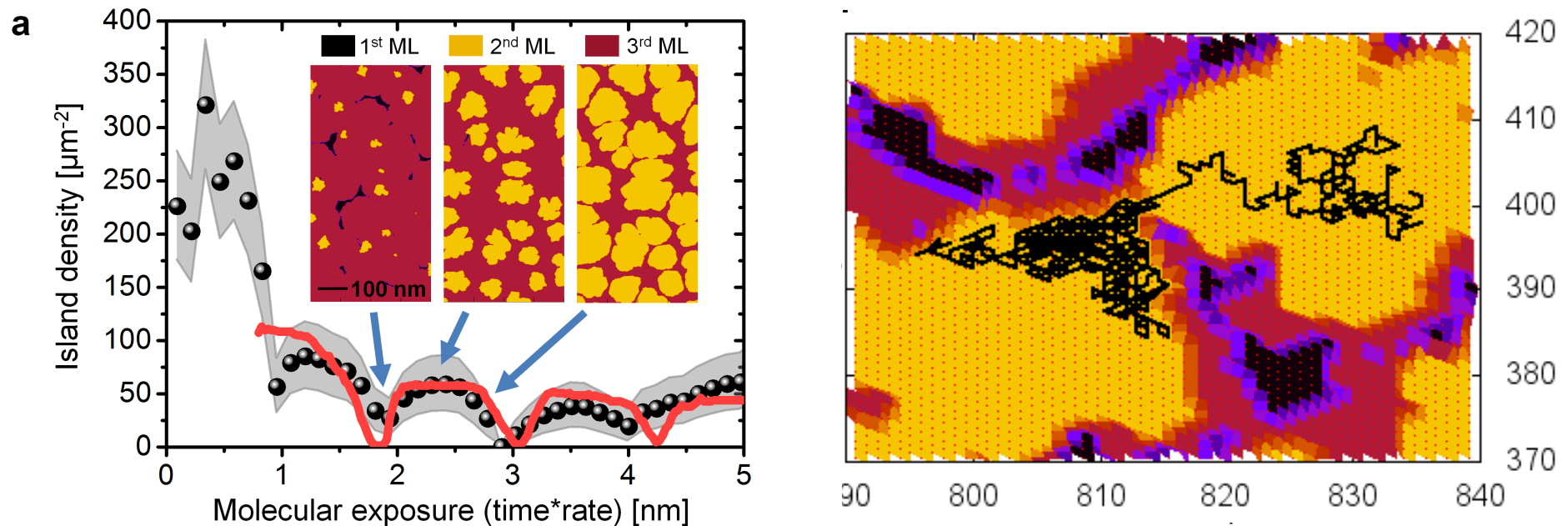


# A7 (Klapp): Achievements 1st period



Growth process of  $C_{60}$  multilayers at surfaces

with A9



## Unravelling the multilayer growth of the fullerene $C_{60}$ in real-time

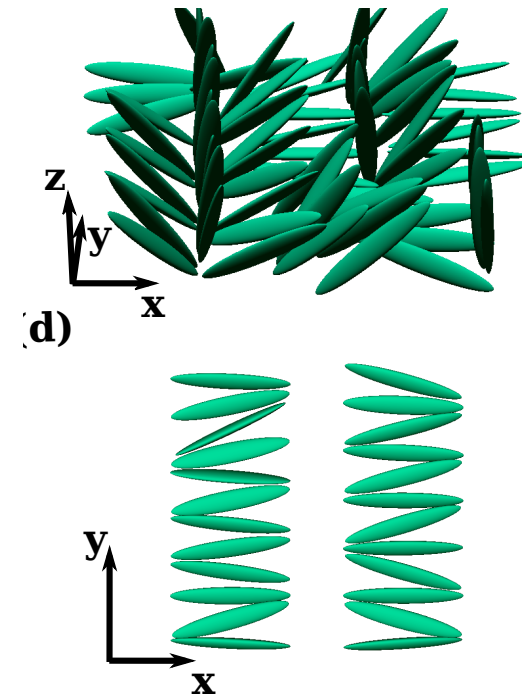
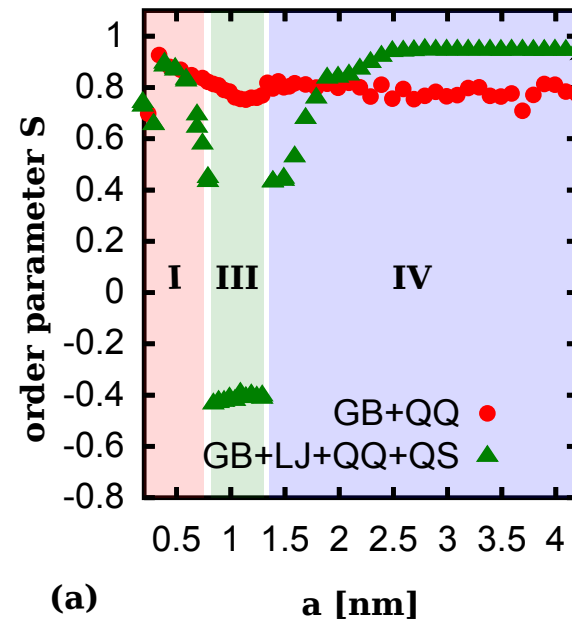
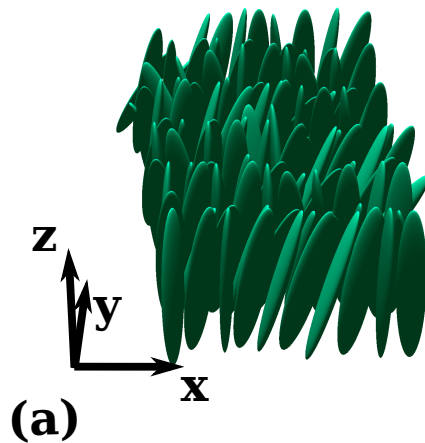
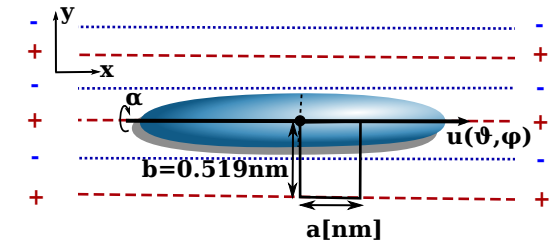
S. Bommel, N. Kleppmann, ..., S.H.L. Klapp, S. Kowarik,  
*Nature Communications* (in press)

## Particle-resolved dynamics during multilayer growth of $C_{60}$

N. Kleppmann and S.H.L. Klapp, *preprint, to be submitted soon*

# A7 (Klapp): Achievements 1st period

Coarse-grained modelling and collective behavior of 6P at ZnO (1010)

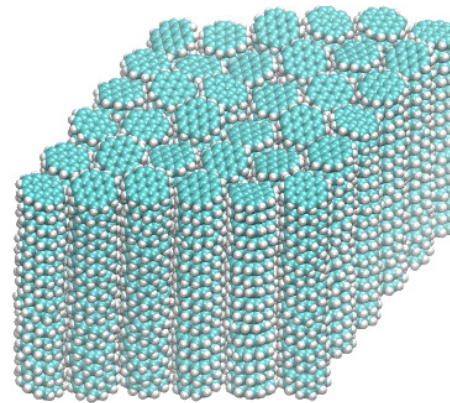
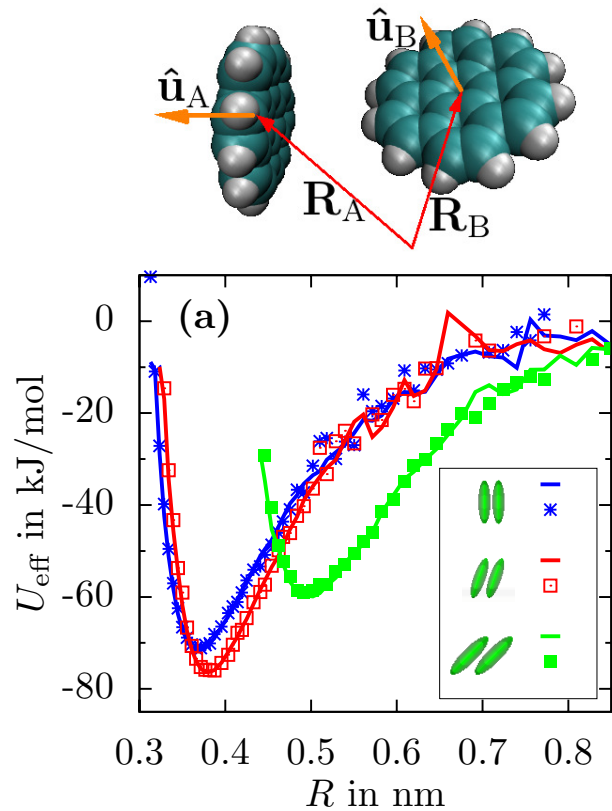


[A scale-bridging model for anisotropic organic molecules at patterned semiconductor surfaces](#)

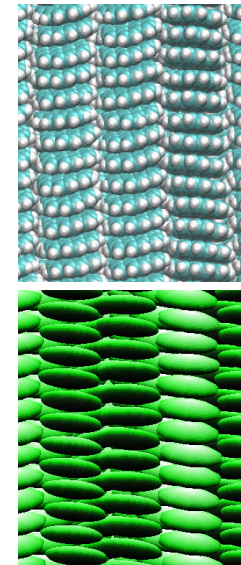
N. Kleppmann, and S.H.L. Klapp, *submitted to J. Chem. Phys.* (2014)

# A1+A7: Joint work in the 1st period

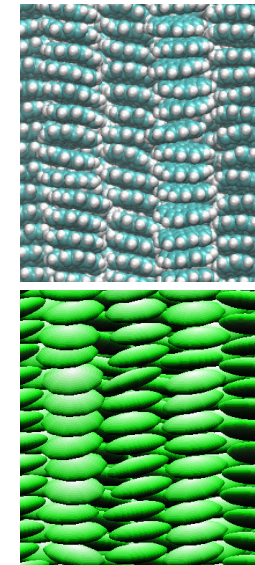
Systematic coarse-graining of anisotropic molecular interactions:  
Reproduction of structure and bulk phase behavior



(a)



(b)



(c)

[Angle-resolved effective potentials for disk-shaped molecules](#)

T. Heinemann, K. Palczynski, J. Dzubiella, and S. Klapp, *J. Chem. Phys.*, submitted (2014).

## Summary 1<sup>st</sup> funding period

Important method development for HIOS systems at finite temperatures - crucial for future work !

- robust atomistic model for polyphenyl
- refined methods to extract long-time diffusion constants from MD
- expandable kMC code (growth, collective behavior)
- “heuristic” and systematically coarse-grained modelling

# Planned work 2<sup>nd</sup> funding period

Main goal: Combine and advance all-atom and coarse-grained simulations to investigate structure formation & growth phenomena in HIOS

## **All-atom MD**

-> Influence of COM polarity, step edges, surface patterns on transport and nucleation



## **Coarse-grained (k)MC, MD**

-> Anisotropic multilayer growth, impact of electrostatics

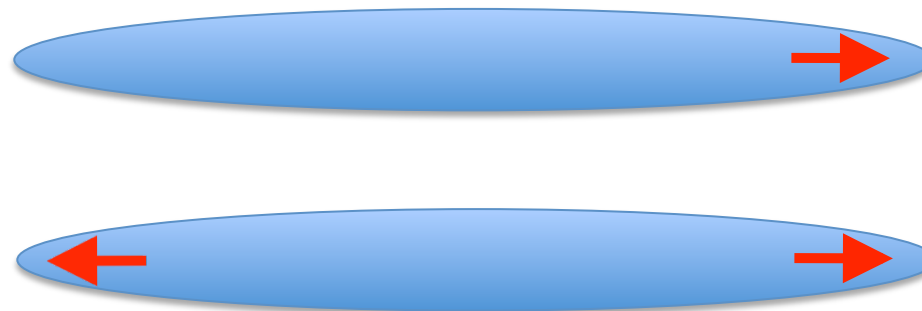
Links:

- anisotropic transport coefficients, energy barriers: all-atom MD-> kMC
- Collective behavior kMC -> all-atom MD

Systems: COM sexiphenyl (**p-6P**) on **ZnO** and derivatives thereof (including local dipoles)

# Questions

- nuclei, island shapes and morphologies (in equilibrium & during growth)
- spatially-varying tilt angle
- impact of different surface modifications and the COM polarity.
- study the (anticipatedly strong) effects of varying the multipole moments of the COM (e.g., local dipoles)



**Inspiration from A3  
(Hecht)**



# Challenges

- Atomistic force-field refinement, explicit polarizability
- Advanced sampling of COM clustering in all-atom molecular dynamics (MD), replica exchange Molecular Dynamics (REMD)
- Identifying appropriate reaction coordinates for coarse-graining
- Ground states and phase diagrams of electrostatically coupled COMS
- Incorporating molecular anisotropy & electrostatics within kMC

# Collaborations within the CRC 951

## Theory

A4 (Heimel): force field parameters from DFT, geometrical single-molecule structure from all-atom MD

A10 (Tkatchenko/Scheffler): force fields for surfaces


B11 (Draxl): electronic surface structure

## Experiment

A5 (Henneberger)

A8 (Koch)

B3 (Blumstengel)

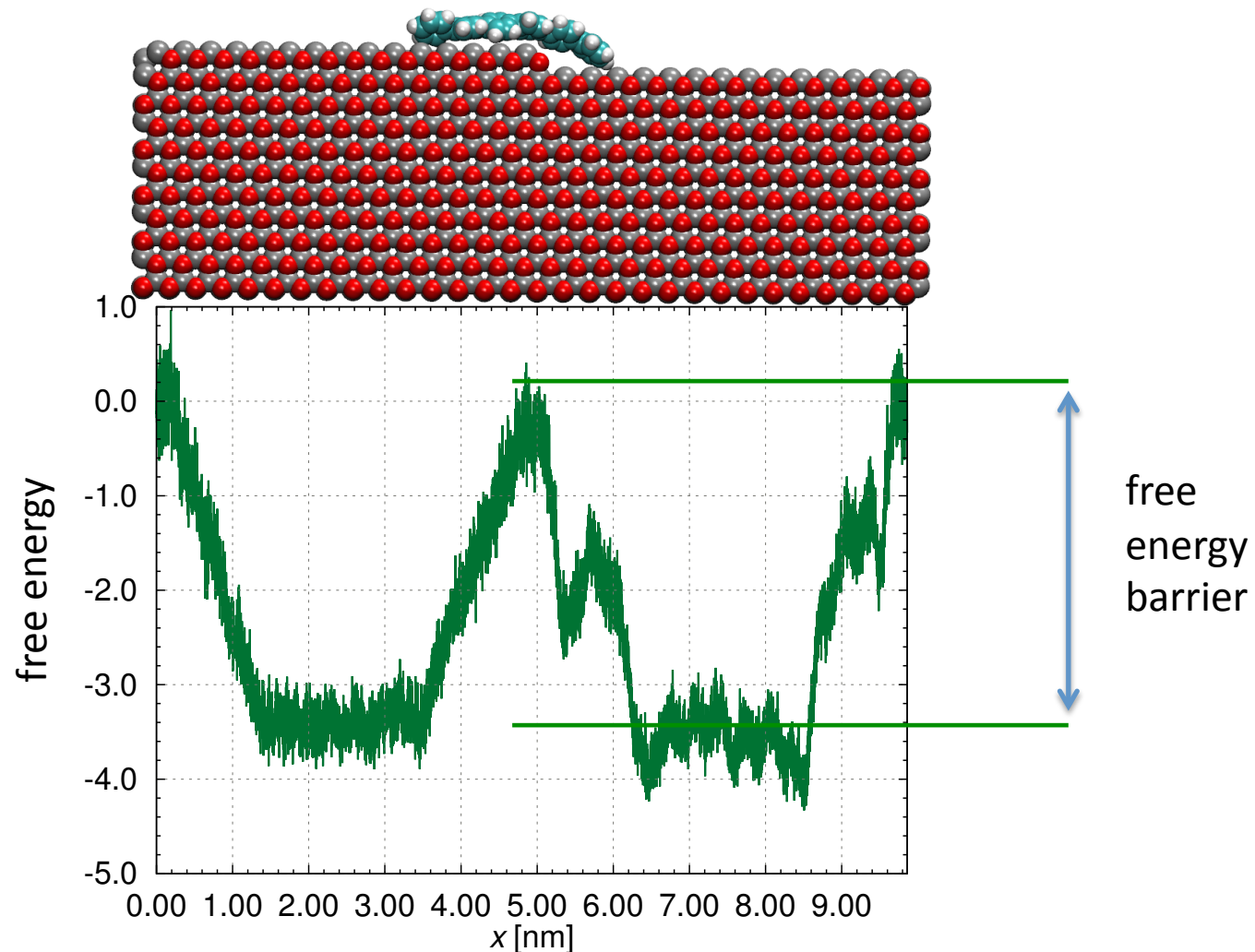


Observation of equilibrium and non-equilibrium aggregated structures (islands, layers, tilt angles, ...)

Z2 (Kowarik/Koch): Time-dependent structures, X-ray

# A1 (Dzubiella): Achievements 1st period

Crossing of a step-edge barrier by a 6P molecule at ZnO



Characterization of step-edge barrier crossing of para-sexiphenyl on ZnO surfaces

K. Palczynski and J. Dzubiella, *in preparation* (2014)