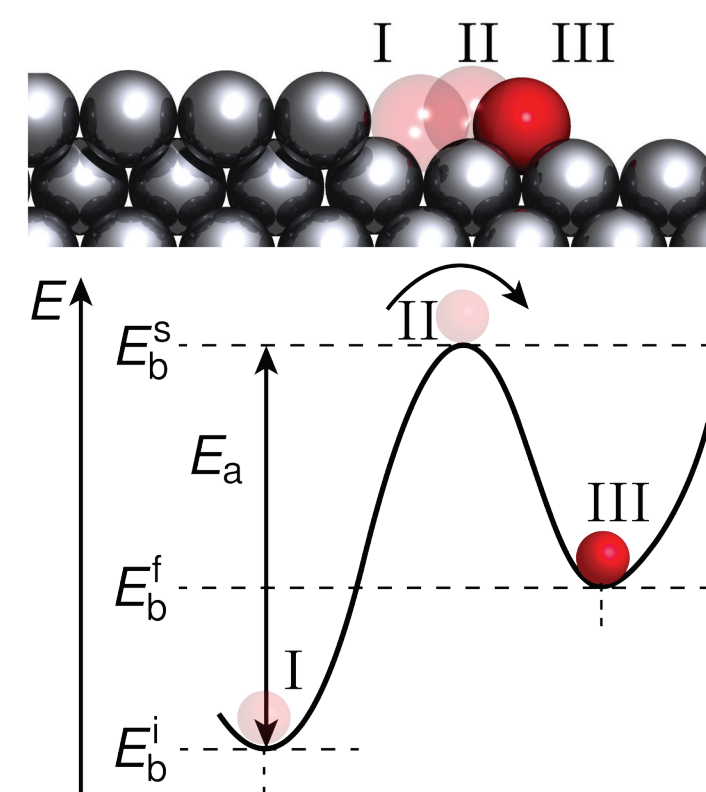# Three-dimensional self-learning kinetic Monte Carlo model

## A. Latz, L. Brendel and D.E. Wolf

**Faculty of Physics, University Duisburg-Essen, and Center for Nanointegration Duisburg-Essen (CENIDE), D-47057 Duisburg, Germany**

## Kinetic Monte Carlo (KMC)

- Dynamical evolution by thermally activated hopping processes.

- Hopping rates: $\nu = \nu_0 \exp\left(-E_a / k_B T\right)$
  $E_a$ = activation energy

- Next process is chosen proportional to its hopping rate.

- Reliability of KMC simulations depends on accurate transition rates.



## Self-learning kinetic Monte Carlo

### SLKMC method [1]:

- Activation energies calculated on-the-fly and stored in a database.

- The local environment is used to identify processes.

- Two dimensional lattice model: $2^{36} \approx 7 \times 10^{10}$ local environments

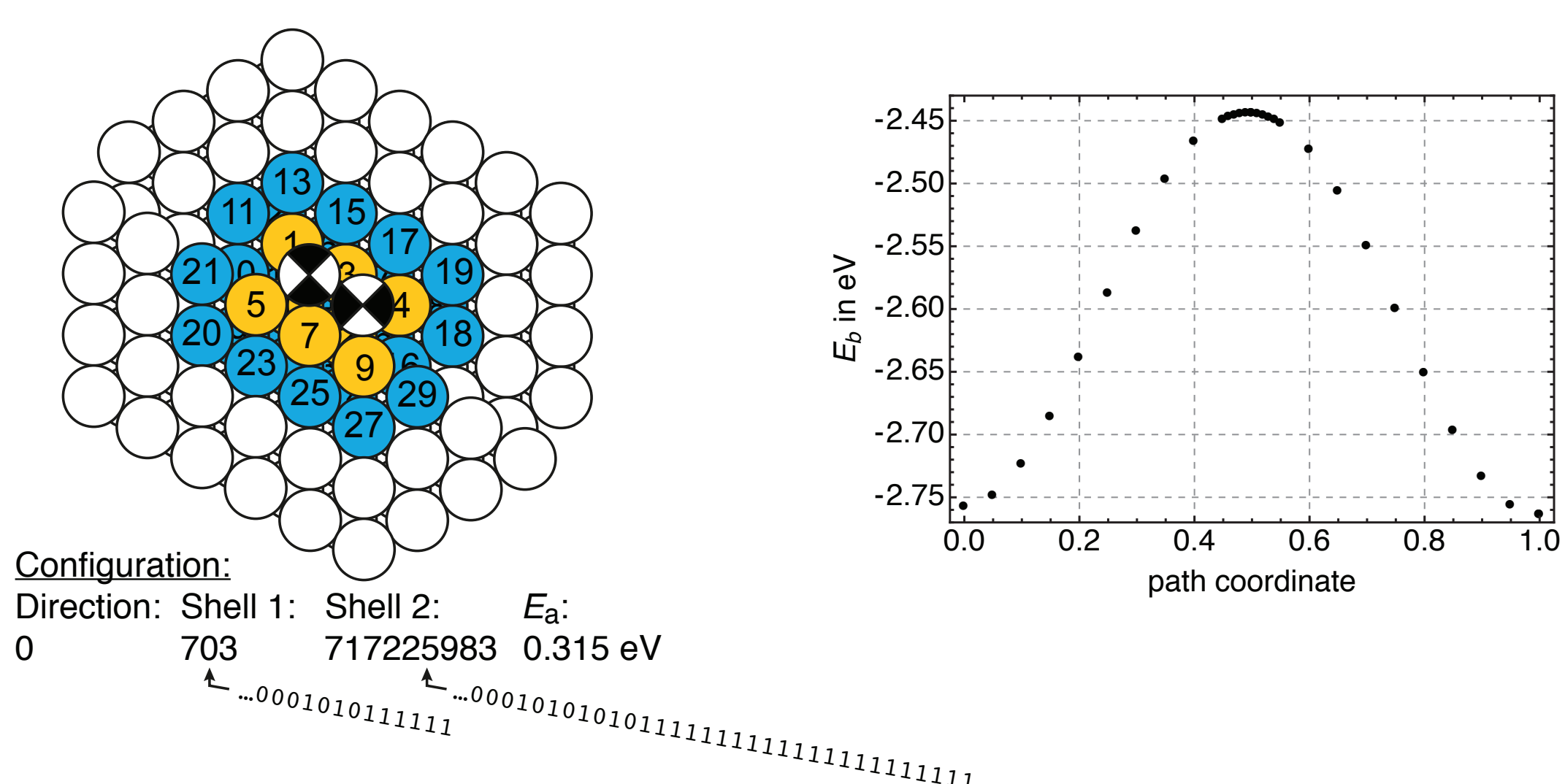### First three-dimensional SLKMC model [2]:

- Three dimensional lattice model: $2^{72} \approx 5 \times 10^{19}$ local environments.

- One $E_a$ calculation approximately 1–10 s on one CPU core.

- On-the-fly $E_a$ calculations reduced by setting up an initial database with likely processes in parallel.

- Atoms restricted to single atom hops between fcc-sites.

- The occupation of the 1st and 2nd neighbor shells of the initial plus final hopping sites define the local environment.



⬤ initial or final hopping site   🟡 1st neighbor shell site   🔵 2nd neighbor shell site
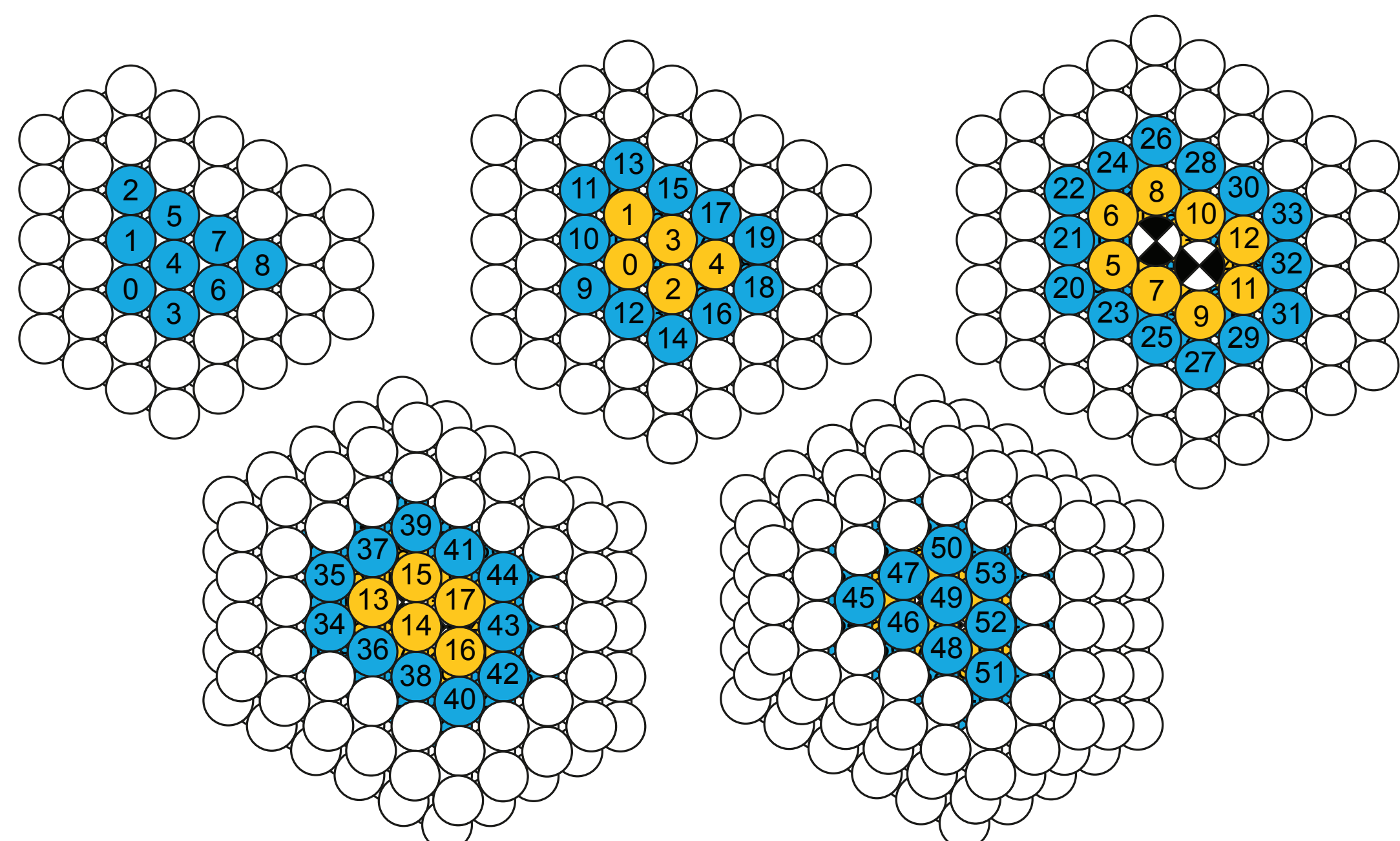
- Configuration encoded in integers: site $i$ occupied ➜ bit $i$ = 1

## Example: Diffusion along step

- $E_a$ calculated with Drag method, using TB-SM potential.



Configuration:
Direction:   Shell 1:   Shell 2:   $E_a$:
0            703        717225983   0.315 eV
  ~0001010111111    ~000101010101111111111111111111111111

## References

[1] O. Trushin *et al.*, *Phys. Rev.* B 72, 115401 (2005)

[2] A. Latz, L. Brendel and D.E. Wolf, *J. Phys.: Condens. Matter* 24, 485005 (2012)

[3] A. Latz, S. Sindermann *et al.*, *Phys. Rev.* B 85, 035449 (2012)

[4] E. Cox *et al.*, *Phys. Rev.* B 71, 115414 (2005)

[5] S. P. Sindermann *et al.*, *J. Appl. Phys.* 113, 134505 (2013)

[6] P. Kuhn *et al.*, *Phys. Rev. Lett.* 94, 166105 (2005)

## Activation energy pre-calculation

- Number of occurring configurations can be tremendous.

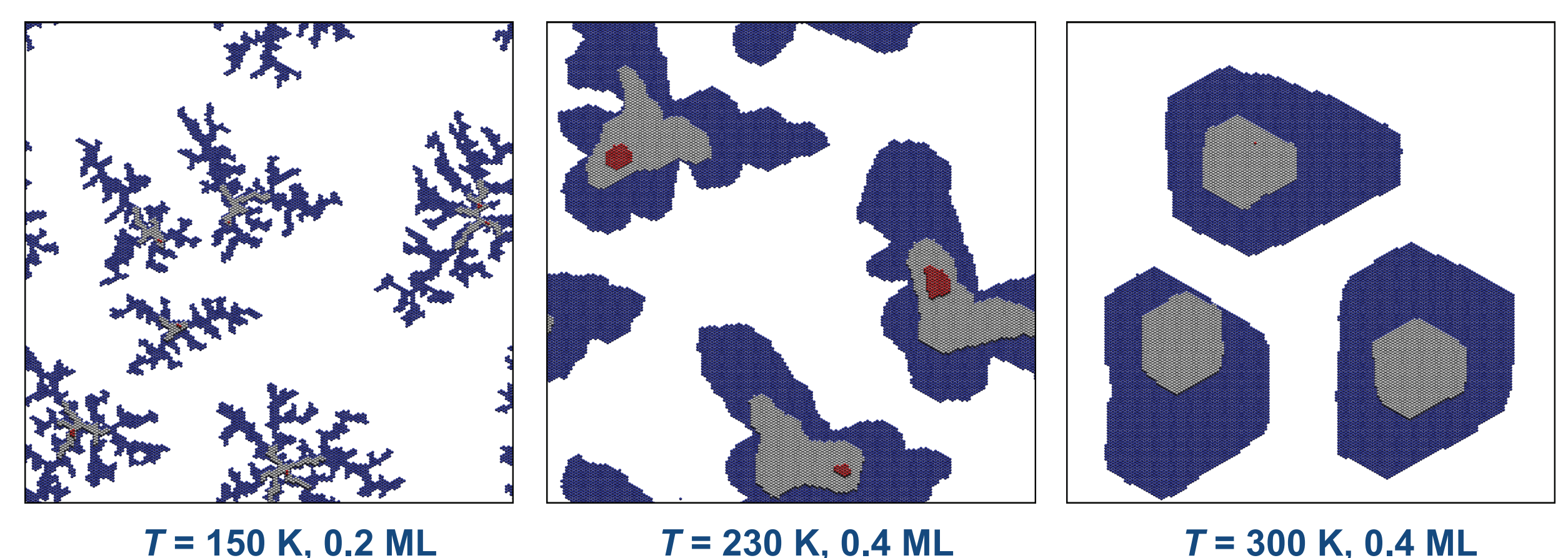- Diffusion of monolayer island on Ag(111):
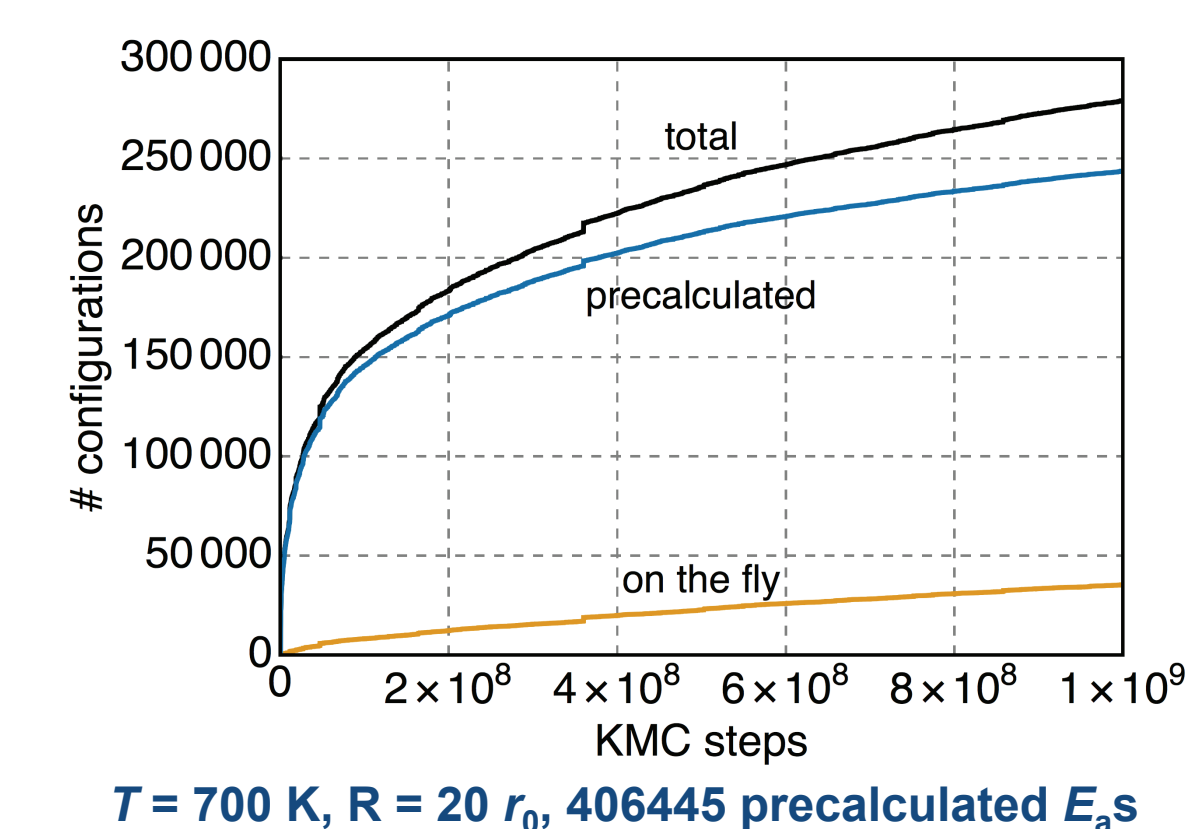


$T$ = 700 K, R = 20 $r_0$, 406445 precalculated $E_a$s

- Initial database:
  - Likely processes gathered with simpler model [3].
  - "Exact" $E_a$s precalculated in parallel.

## Applications

### Homoepitaxial film growth on Ag(111)

- Atoms are deposited with a constant rate ($F$ = 10 ML/s) on a 50x50 nm$^2$ Ag(111) substrate.



$T$ = 150 K, 0.2 ML          $T$ = 230 K, 0.4 ML          $T$ = 300 K, 0.4 ML

- Dendritic islands at $T$ = 150 K

- With increasing temperature, periphery diffusion becomes fast enough that dense islands can form.

- Quantitative agreement with experiments [4] emergent from a correct microscopic treatment.

### Electromigration-induced void and island drift anisotropy

- Electromigration: Directed motion of atoms driven by high electric fields.

- Effective force: $\vec{F}_{EM} = Z^* |e| \vec{E} = Z^* |e| \rho \vec{j} = const$

- $E_a$ variation: $\Delta E_{EM} = -\vec{F}_{EM} \cdot \vec{x}_{is}$
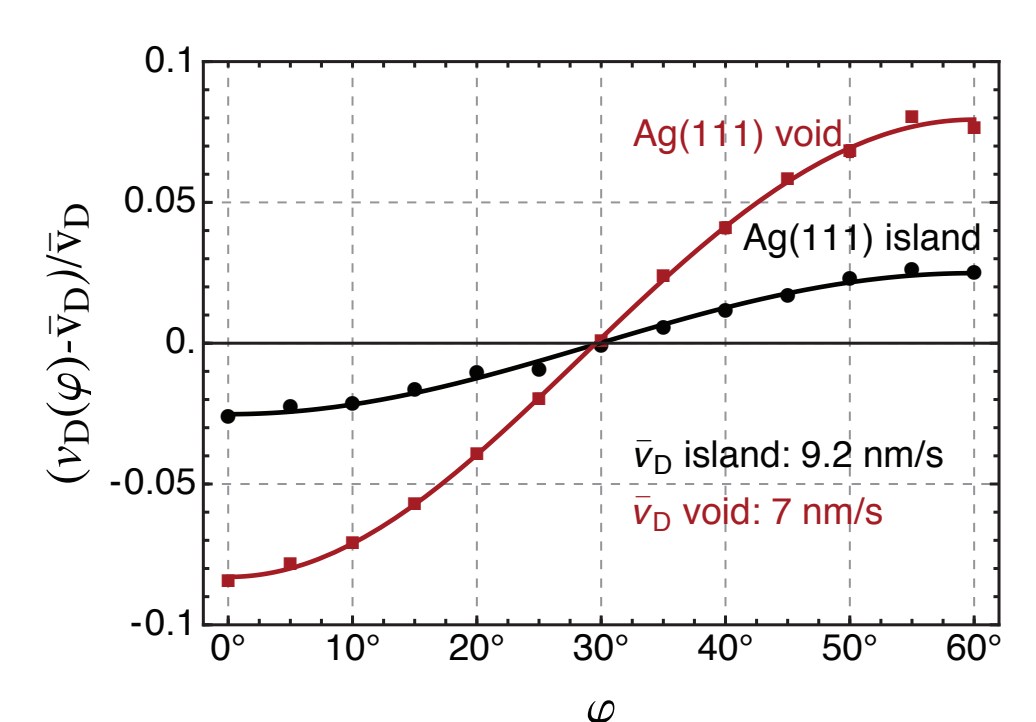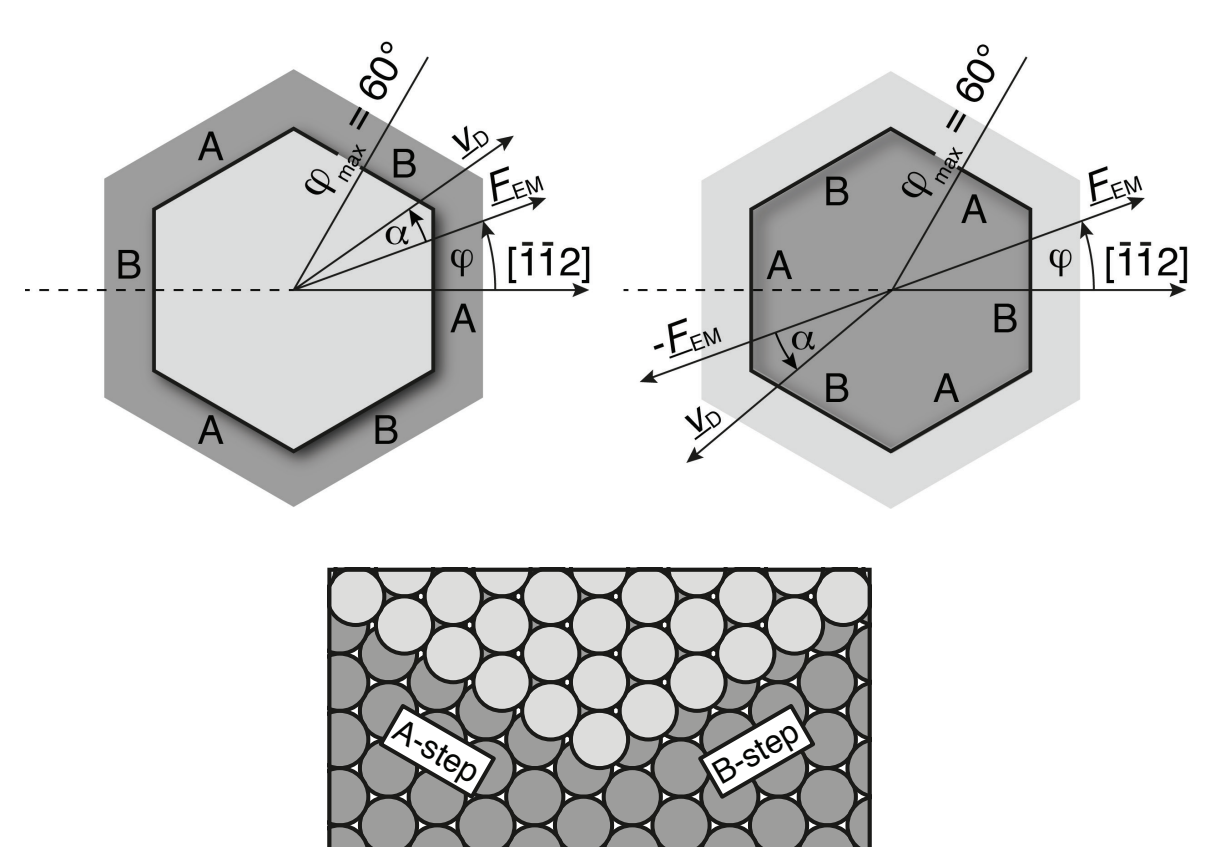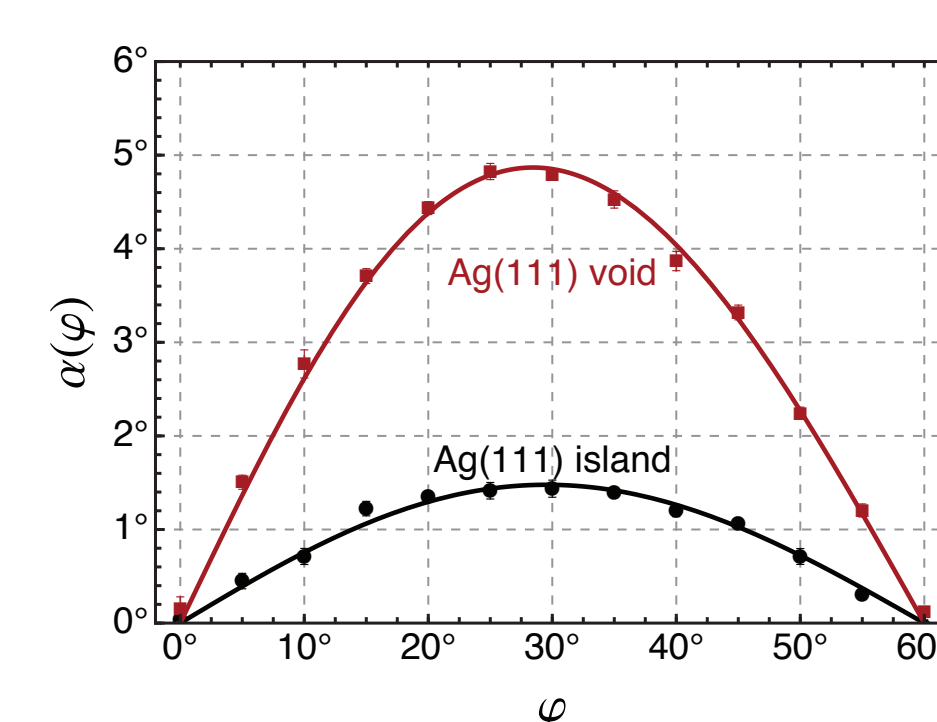
- Monolayer islands and voids on Ag(111)
  - $F_{EM}$ = 0.002 eV/nm ≙ $j$ = 5 × 10$^8$ A/cm$^2$
  - $T$ = 350 K: facetted, hexagonal shape
  - Threefold symmetry (A- and B-steps)

- Measured quantities: $|\underline{v}_D|$ and angle α between $\underline{v}_D$ and $\pm\underline{F}_{EM}$

- $|\underline{v}_D|$ and α averaged over 20+ trajectories.





- Periphery diffusion

- Island and Void (111):
  - $|\underline{v}_D|$ largest in B-step direction.
  - α > 0, preferred drift in B-step direction