Computational Materials Science

The Computational Materials Science group at Saarland University uses computer simulations to rationalize the behavior of materials from elementary principles.

Particular research interests include
- Unraveling friction mechanisms
- Contact mechanics and adhesion
- Design of interatomic potentials
- Modeling redox processes with atoms
- Phase transformations in phase-change materials and bulk-metallic glasses

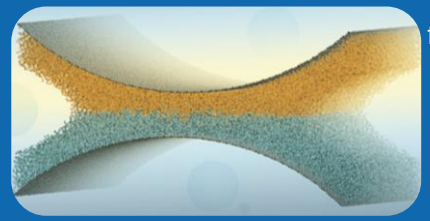
EEIGM Teachers/Researchers

Martin Müser

Expertise: Atomistic-computer simulation, boundary-value methods, statistical mechanics

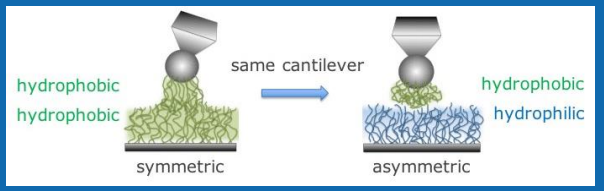
Teaching: Physics, computer simulation & mathematical methods in materials physics

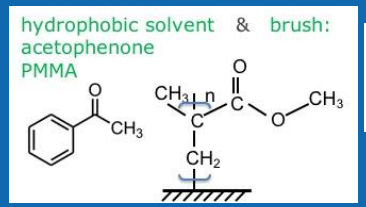
Dissipation mechanisms in bio-inspired contacts



from atomistic interaction via coarse-grained models

from coarse-grained models to prediction and design

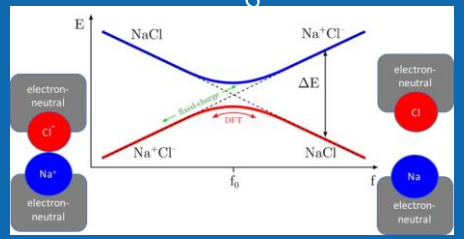




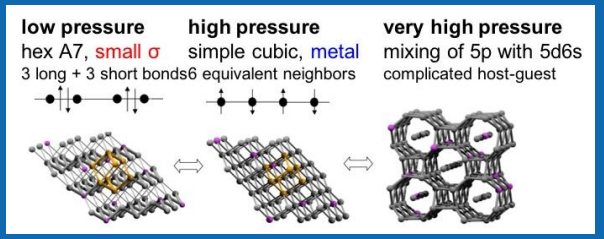
$$V = V_{sr} + \sum_i \frac{k_i}{2} Q_i^2 + c_i Q_i + \sum_{j>i} \frac{1}{4\pi\varepsilon_0} \times \frac{Q_i Q_j}{R_{ij}} + \frac{k_{ij}^{\text{bond}}}{2} q_{ij}^2$$

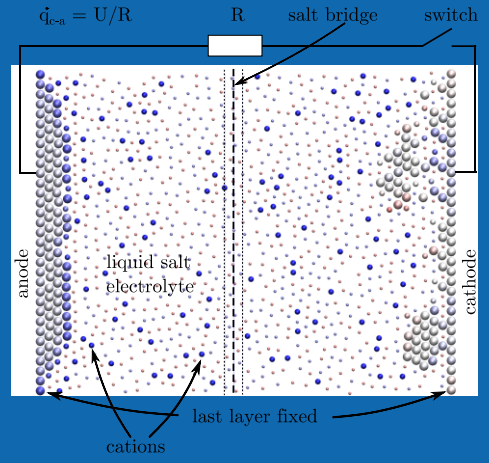
simulation

coarse-graining of electronic structure



explaining response of matter to extreme conditions (pressure)





unraveling redox-induced phenomena from elementary principles