Applied Theoretical Physics – Computational Physics

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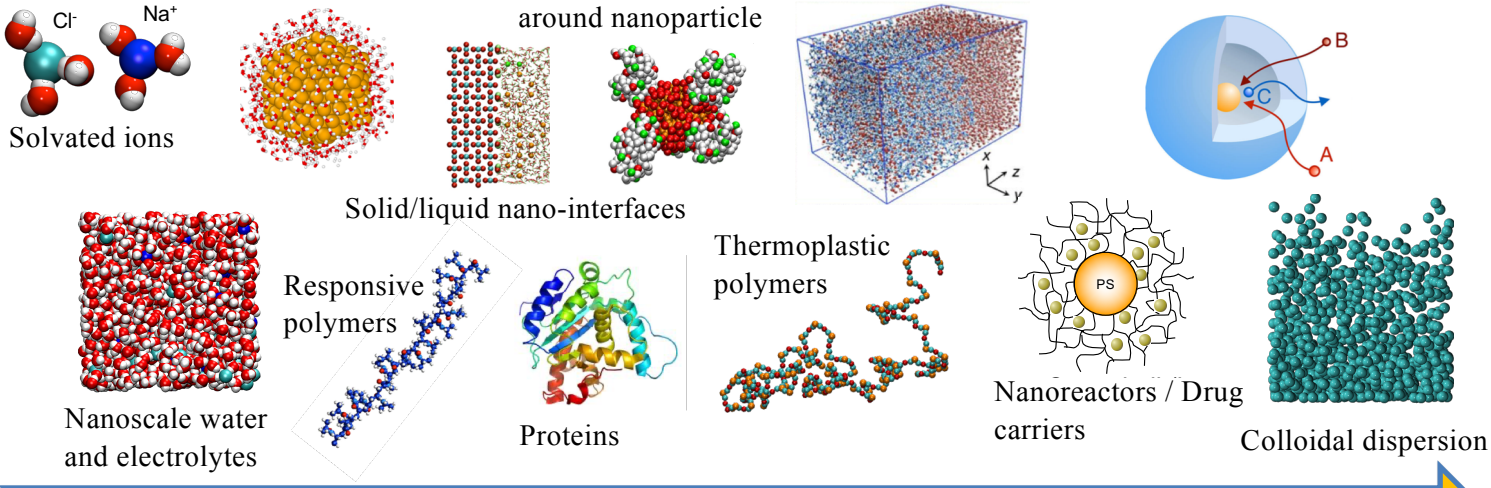
UNI FREIBURG

Research:

- Computer simulations and theoretical modeling of soft functional materials
- Goal: establish (microscopic) structure-property-function relationships and design rules

Systems / Materials we simulate and study



Multiscale Methods (all based on classical Hamiltonians)

Molecular Dynamics (Newton, all-atom) $m\ddot{\mathbf{r}}_i = \sum_j \mathbf{F}_{ij}$	Mesoscopic Dynamics (Langevin, coarse-grained) $m\ddot{\mathbf{r}}_i = -\xi m\dot{\mathbf{r}}_i + \sum_j \mathbf{F}_{ij} + \theta_i$	(kinetic) Monte-Carlo, Reaction-Diffusion simulations $P(x \to x^*) = \min\left\{1, \frac{P(x^*)}{P(x)}\right\}$	**Computer ‚experiments'**
Liquid State Theory / Statistical Mechanics	Polymer Physics / Electrostatics / Nonequilibrium transport	Thermodynamics / Continuum Mechanics / Hydrodynamics	**Theoretical Physics**

Environment and Perspective

HZB Helmholtz Zentrum Berlin

- *Team Freiburg:* 4 postdocs, 2 PhD-students, 4 Master students; *Team Berlin:* 2 postdocs, 3 PhD-students
- *Interdisciplinary Research*: Physics meets Computational Science, Chemistry, Molecular Biology, Applied Mathemathics & Engineering
- *International Collaborations*: Helmholtz-Zentrum & HU Berlin, Sorbonne Université Paris, Imperial College London, UC San Diego, University of Malaga, Granada, etc.
- *Education & Job Perspectives*: Research & Development in Computational Material Science (Emerging Branch of Industry); Data Science and Analytics; Finance and Risk

Lectures / Labs

- In SoSe 21: Master Course on Computational Physics for Materials / Oberseminar Computational Soft Materials
- Master Laboratory Applied Physics: Nano Tug-of-war Computational Exploration of Polymer Elasticity