Computational Quantum Field Theory (CQT)

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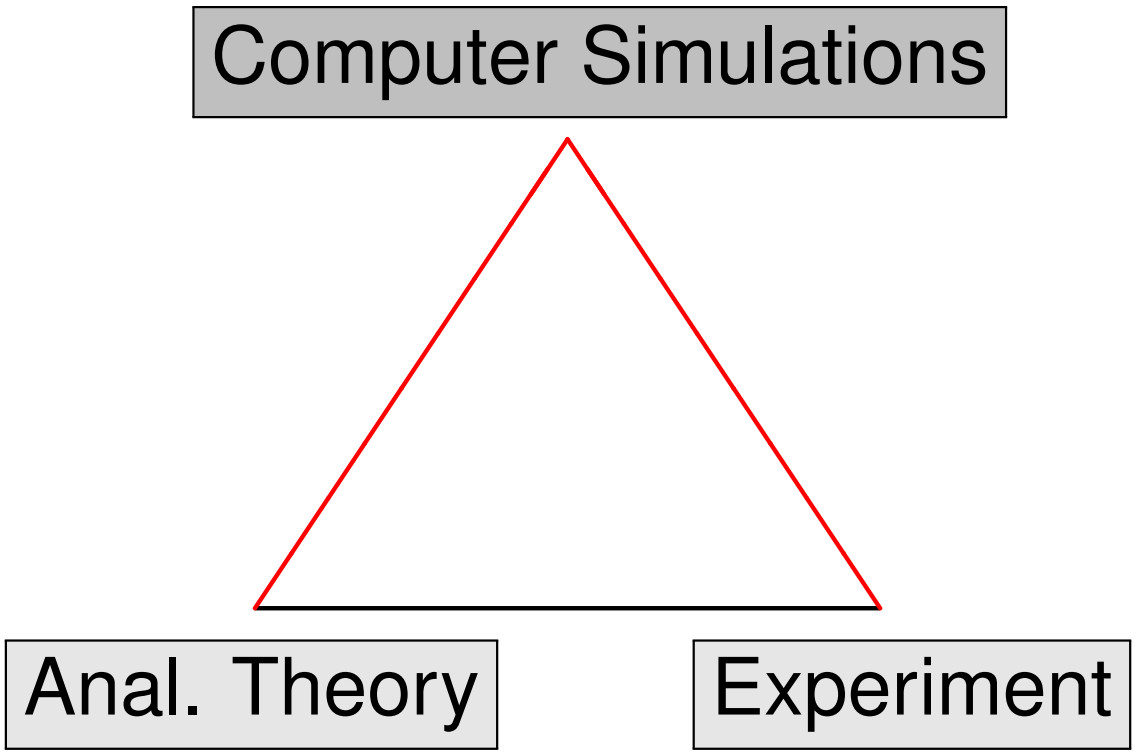
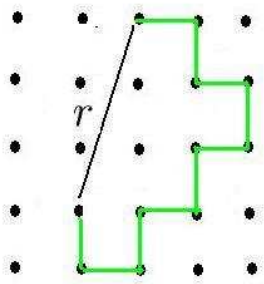
Methodologies

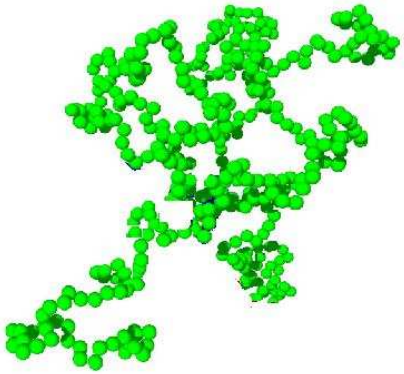


Advanced Monte Carlo (MC) and Molecular Dynamics (MD) computer simulations

Polymers as Self-Avoiding Random Walks (SAWs)



N steps



$N+1$ monomers

- SAW = random walk (RW) that is *not* allowed to cross itself
- Average end-to-end distance $\langle R_{ee} \rangle \propto N^{\nu_{\mathrm{SAW}}}$ with "critical" exponent $\nu_{\mathrm{SAW}} \approx \frac{3}{d+2} \geq 1/2 = \nu_{\mathrm{RW}}$,
- Number of polymer (SAW) conformation $Z_N = c\,\mu^N N^{\gamma_{\mathrm{SAW}}-1}$

Polymer Models in the Continuum

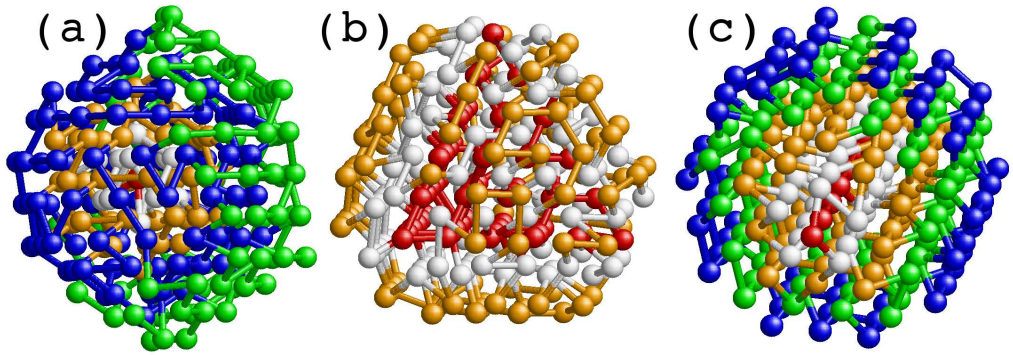
Lennard-Jones (LJ) + bond potential:

$$E = \frac{1}{2}\sum_{\substack{i,j=1 \\ i\neq j}}^{N} 4\epsilon[(\sigma/r_{ij})^{12} - (\sigma/r_{ij})^{6}] + \sum_{i=1}^{N-1} V_{\text{bond}}(r_{ii+1})$$

with

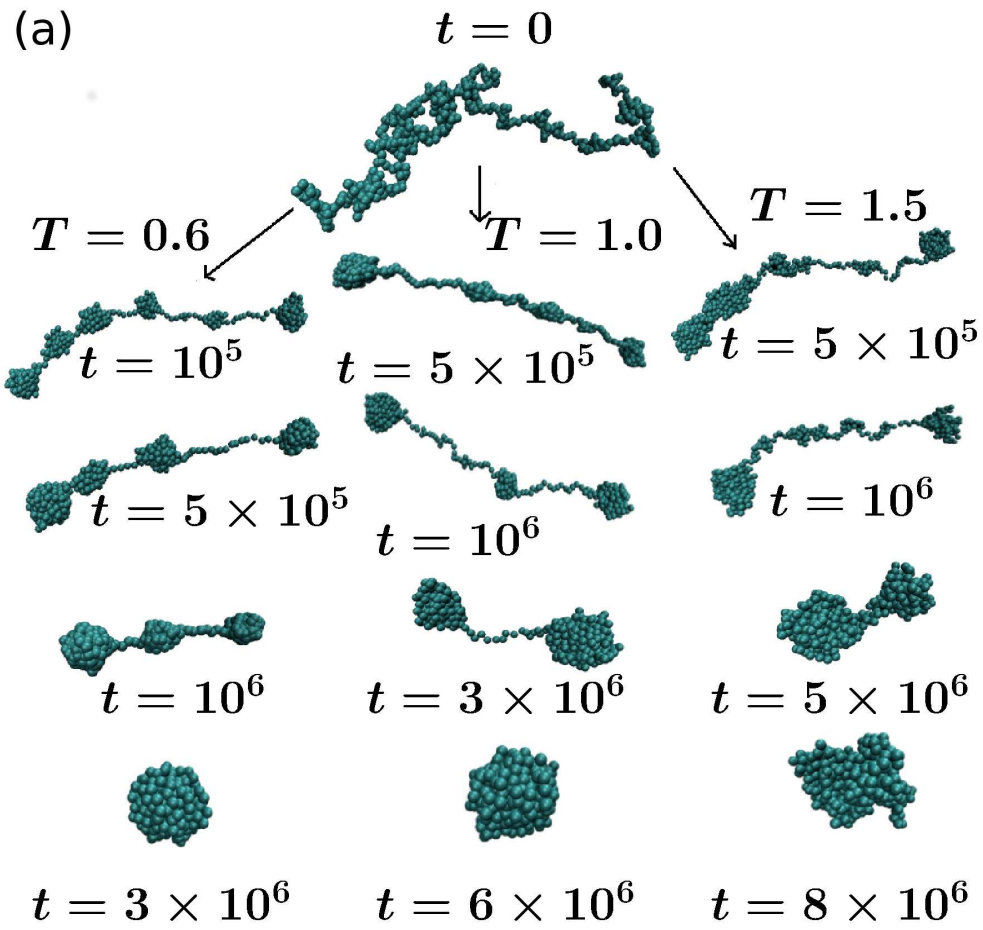
$$V_{\text{bond}}(r_{ii+1}) = -\frac{K}{2}R^2 \ln\{1 - [(r_{ii+1} - r_0)/R]^2\}.$$

Ground-state “crystals”, similar to atomic LJ clusters:

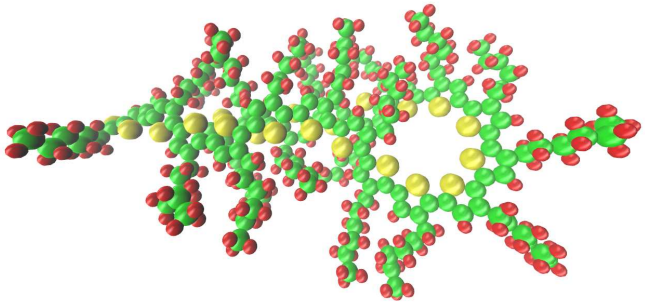
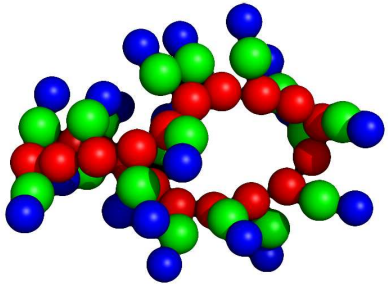
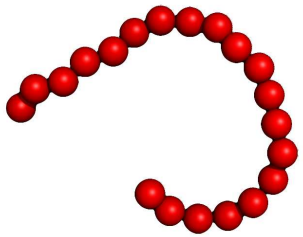


$N = 234$: icosahedral tetrahedral decahedral

Polymer Collapse Kinetics



Polymers from All-Atom to Coarse-Grained Models

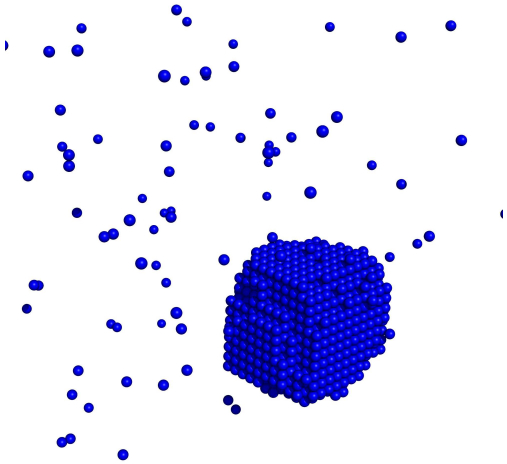




P3HT: Poly(3-hexylthiophene)

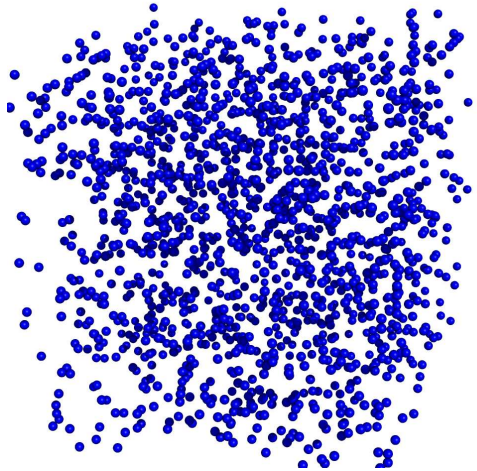
Adsorption of P3HT on gold surface in ultrahigh vacuum: Computer simulations in comparison with experiments done at University Halle

Polymer Aggregation versus Particle Condensation

Condensed



Evaporated



Balancing interface (free) energy vs fluctuations

energy vs entropy

Further Research Topics

- Disordered systems (spin glasses, long-range correlated disorder, . . .)
- Method development (population annealing, long-range interactions, . . .)
- Active matter systems
- Machine learning

Perspectives

- DFG Sonderforschungsbereich/Transregio SFB/TRR 102 *Polymers under Multiple Constraints: Restricted and Controlled Molecular Order and Mobility* with integrated Research Training Group (iRTG) (with Univ. Halle)
- German-French PhD College (exchange programme with Nancy, Coventry and Lviv)
- Graduate School *BuildMoNa – Building with Molecules and Nanoobjects* (with Chemistry, Biochemistry)
- International Max Planck Research School (IMPRS) *Mathematics in the Sciences* (with Math., MPI MIS)
- Cooperation with PhD school in Krakow
- EU COST action EUTOPIA

Infos

- CQT Homepage:
  http://www.physik.uni-leipzig.de/cqt.html
- CQT Report 2018:
  http://www.physik.uni-leipzig.de/~janke/research/reports.html
- 20th International Workshop on *New Developments in Computational Physics "CompPhys19"*:
  28 – 30 November 2019
  http://www.physik.uni-leipzig.de/~janke/CompPhys19
  $\longrightarrow$ Programme/Abstracts of Talks