TECHNISCHE UNIVERSITÄT DRESDEN

DRESDEN concept

Chair of Material Science & Nanotechnology
Institute for Material Science

Multiscale Simulation Framework for Functional Polymers

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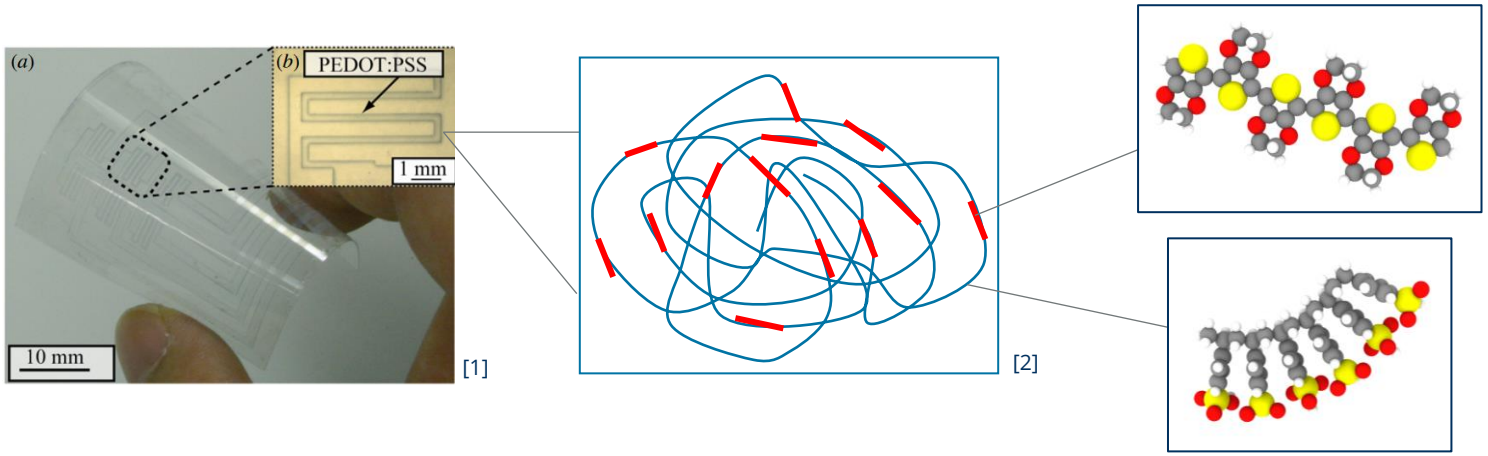
Motivation

- **How can the functional properties of a polymer be predicted for an application?**

  → Determination of functional parameters from atomistic level upwards

- **Challenges:**
  - Property optimization based on structural analysis & local atomistic conditions



[1] [2]

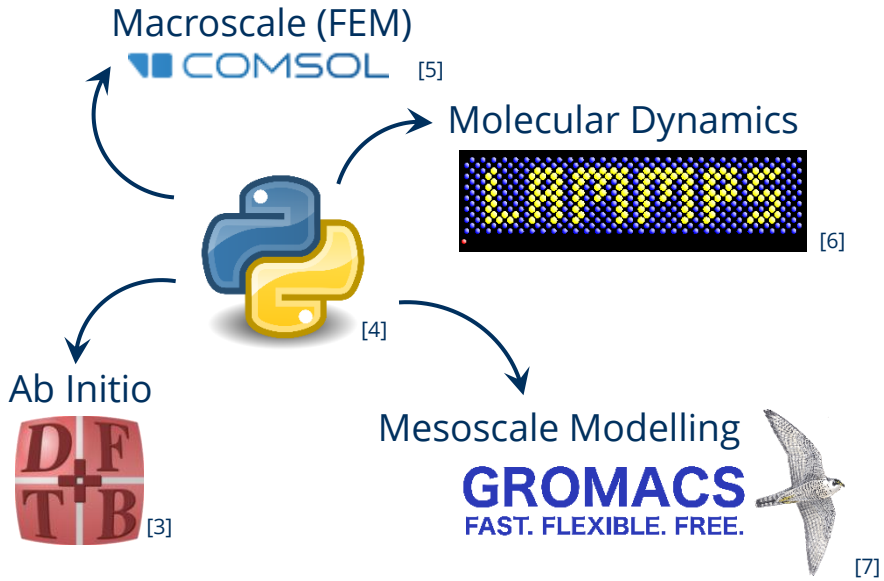
Hierachical property relations! → Example: Strain gauge

[1] S. Takamatsu et al., J. Micromech. Microeng. 2010, 20, 6
[2] Based on: U. Lang, E. Müller, N. Naujoks, J. Dual, Adv. Funct. Mater. 2009, 19, 1215

Introduction

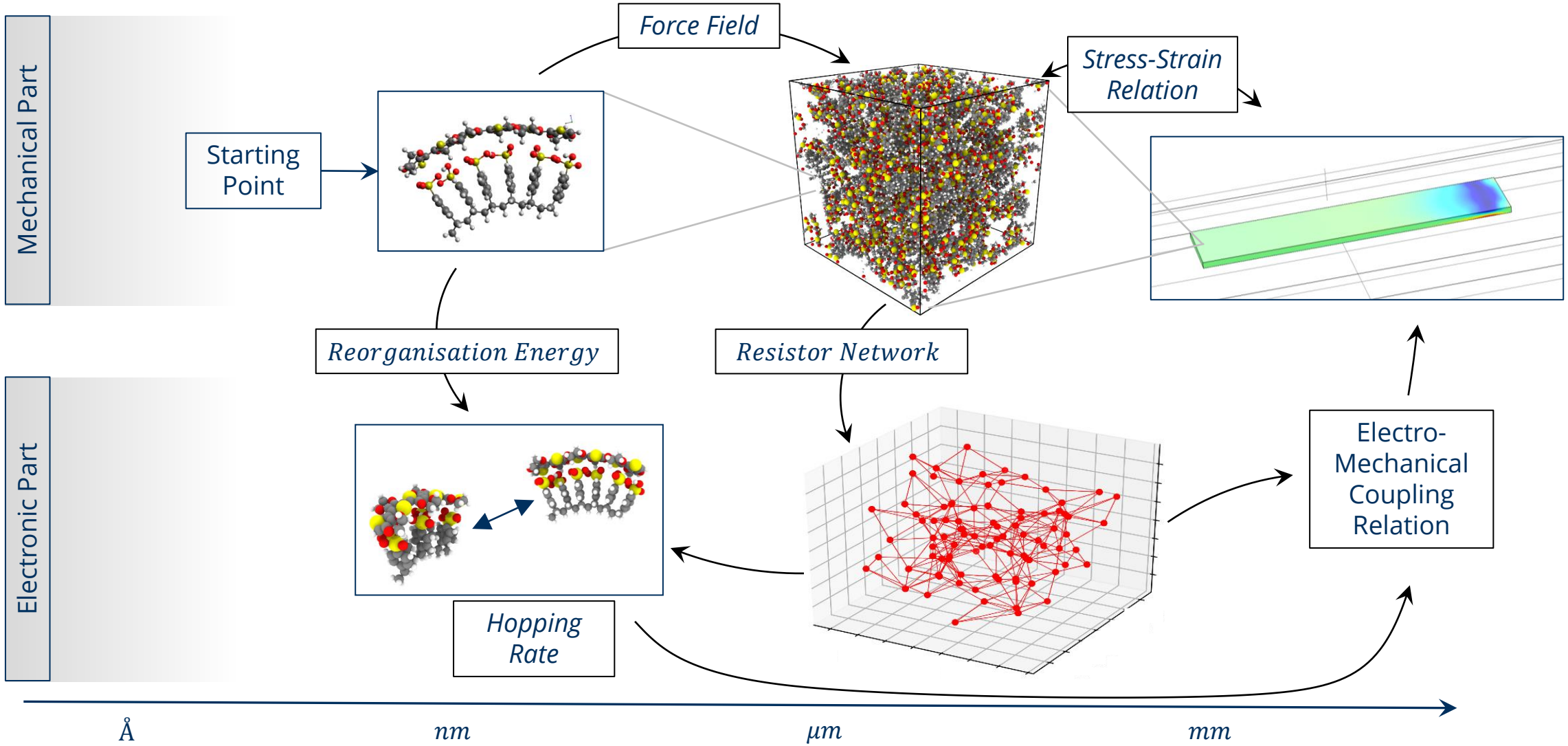
- Combining advantages of (*open source*) modelling & simulation software with **simulation framework**
  - Python programming language as control unit
  - Includes pre- and post processing
  - Flexible & extendable

- **Starting point:** Poly-3,4-ethylenedioxythiophene (PEDOT)
  - Wide researched polymer
  - Many modifications



[3] https://dftbplus.org/fileadmin/_processed_/e/8/csm_DFTB-Plus-Icon_06_f_1200x1200_9121b134be.png
[4] https://upload.wikimedia.org/wikipedia/commons/0/0a/Python.svg
[5] https://upload.wikimedia.org/wikipedia/commons/2/28/Comsol_logo.svg
[6] https://lammps.sandia.gov/movies/logo.gif
[7] https://developer.nvidia.com/blog/wpcontent/uploads/2020/02/gromacs_logo1_centered.png

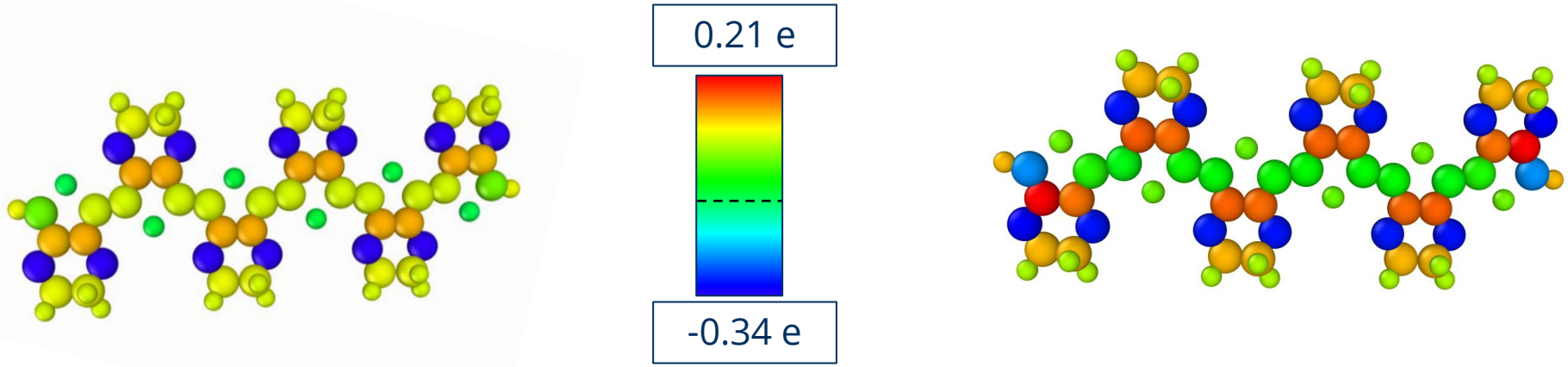
Multiscale Electronic-Mechanical Coupling



Molecular Build Up

What do we need fundamentally for simulating our polymer system?

- Estimation of **force field**
  - Charges from *Dreiding* [8] force field vs. *ab initio* method



- Inter-molecular energy: Lennard-Jones Potential $E(r) = 4\varepsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$

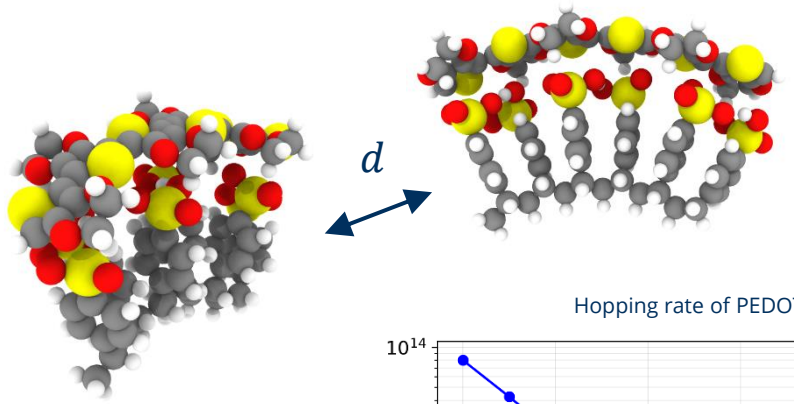
- **RVE:** Adjustable volume fraction of PEDOT & PSS chains → semi-crystalline, amorphous

[8] S. L. Mayo, B. D. Olafson, W. A. Goddard III, J. Phys. Chem. 1990, 94, 8897

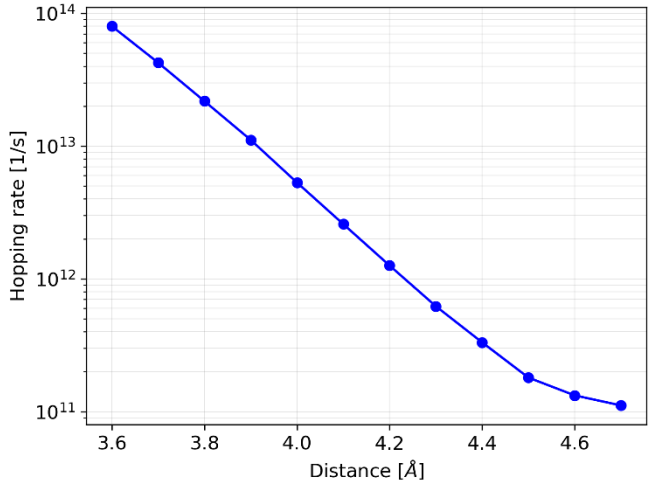
Calculation of Individual Resistors

Hopping rate: $k = t^2 \left(\frac{\pi}{\hbar^2 k_B \lambda T}\right)^{\frac{1}{2}} \exp\left(-\frac{\lambda}{4 k_B T}\right)$ [9], [10]

t – Transfer integral, λ – Reorganisation energy



Hopping rate of PEDOT-Pair



Mobility: $\mu = \frac{e k d^2}{2\, n_D k_B T}$ [11]

d – Distance, n_D –Dimension

- With Ohm's law

Resistivity: $\boldsymbol{\Pi}\, \sigma = \Delta\rho(\mu)$

$\boldsymbol{\Pi}$ – Piezoresistive coupling matrix

- Describes macroscopic electronic-mechanical coupling

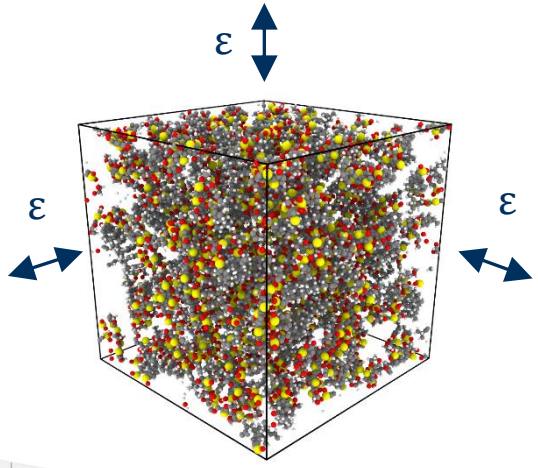
Using hopping rate to describe piezoresistive coupling!

[9] F. Günther, S. Gemming, G. Seifert, J. Phys. Chem. C 2016, 120, 9581
[10] D. Cagardová et al., Acta Chimica Slovaca 2018, 2, 83
[11] S.-H. Wen, A. Li, J. Song, W.-Q. Deng, K.-L. Han, W.A. Goddard III, J. Phys. Chem. B 2009,113, 26, 8813

Electronic-Mechanical Coupling: Network Approach

Elastic Network:

- Deformation of Representative Volume Element (RVE) in different directions

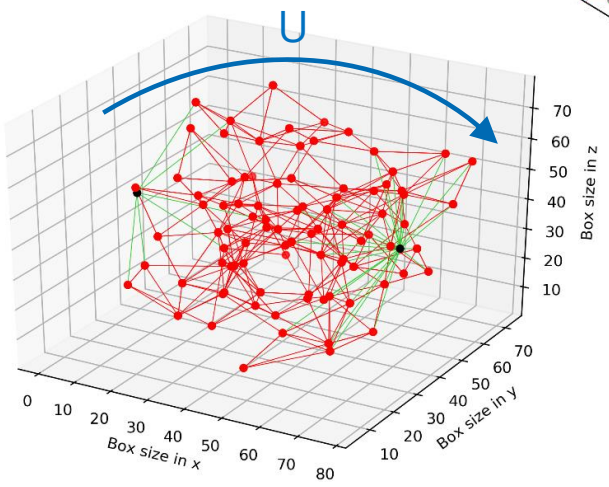


- Determination of anisotropic elastic properties

Electronic Network:

- Construction of network
  - Based on chain positions & distances between chains
- Calculation of electrical resistance in load direction [12]

$$R_{direction} = \frac{U}{I}$$



[12] H. A. Knudsen, S. Fazekas, Journal of Computational Physics 2006, 211, 700

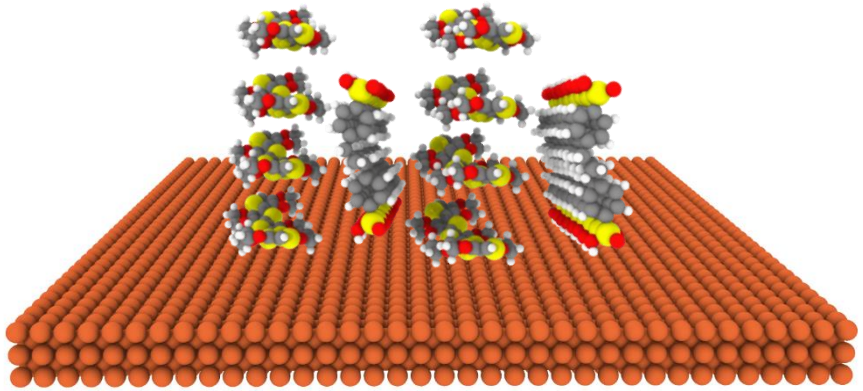
Analysis of resistance over all time steps of MD simulation!

Summary & Outlook

Summary:

- Molecular Dynamics (MD) simulations as fundamental basis for polymer structure
- Ab initio method is chosen to describe resistance between chains
- Combination of MD simulation & ab initio simulations for piezoresistive coupling
- Elastic properties from MD simulations

→ Input for **macroscale simulations** (FEM)



Outlook:

- Implemention of microscopic chain structures
- Framework transfer to different functional properties → Gas sensor [13]

[13] A. Marutaphan, Y. Seekaew, C. Wongchoosuk, Nanoscale Research Letters 2017, 12, 90

Thank your for your attention!