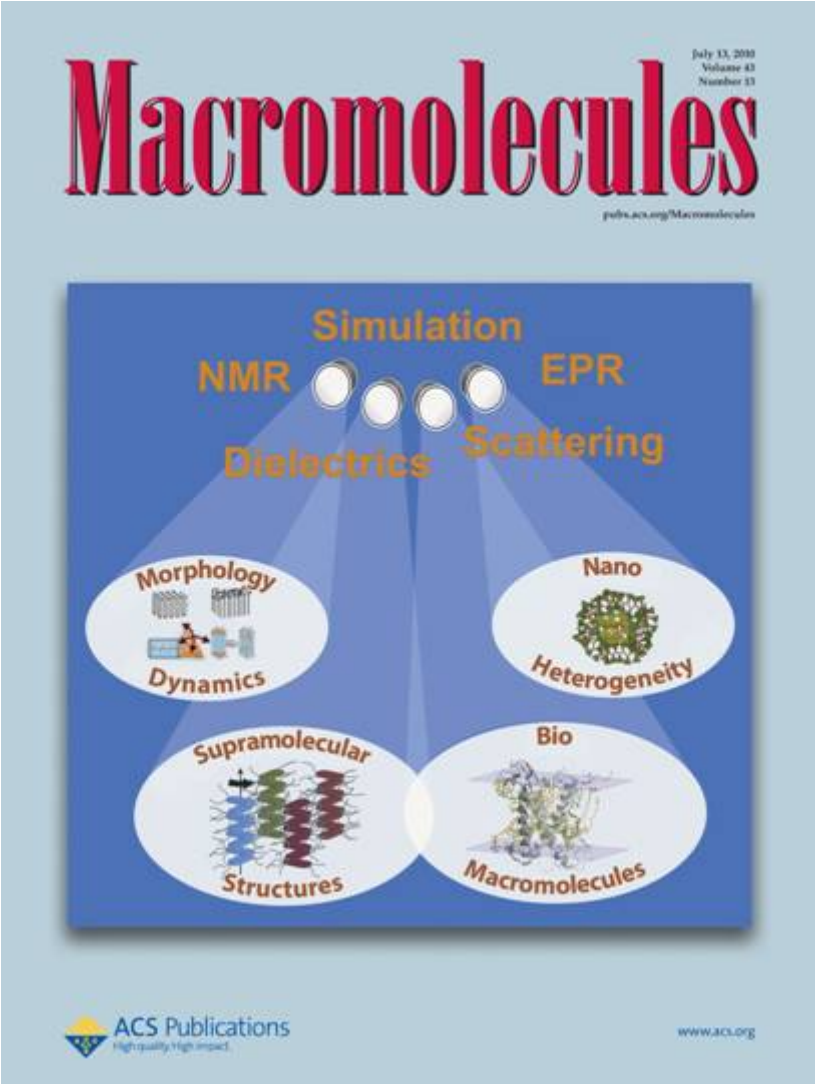
Aufklärung von Struktur und Dynamik:
Skalenübergreifend **(HWSp)**

Rolle der Charakterisierung
bei der Entwicklung neuer Materialien (KS)

- **Interplay of Structure and Dynamics**
- **Synthetic vs. Bio-macromolecules**
- **Multi-Technique Approach**

Functional Materials require Multi-Technique Approach



The delicate **interplay** of structure and dynamics in macromolecular and supramolecular systems leads to increasing **complexity** and **functionality**.

This poses considerable **challenges** for their physical **characterization**.

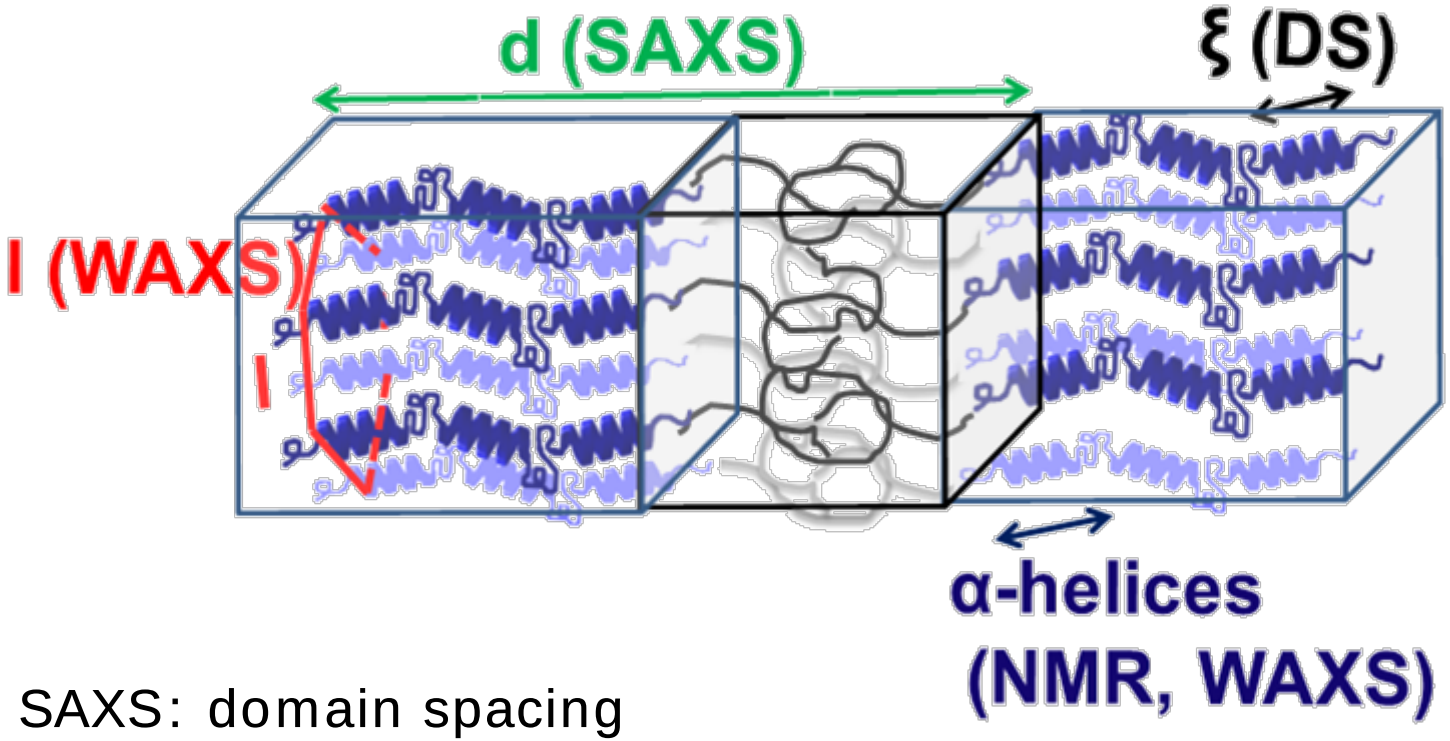
No experimental or theoretical / simulation approach **alone** can provide **complete** information.

Instead, a **combination of techniques** is called for and conclusions should be supported by results provided by as many **complementary methods**

H. W. Sp. Interplay of Structure and Dynamics in Macromolecular and Supramolecular Systems, *Macromolecules*, **43**, 5479–5491 (2010)

Self-assembly and Dynamics of Polypetides

Scheme of a lamellae forming polypeptide-coil diblock copolymer



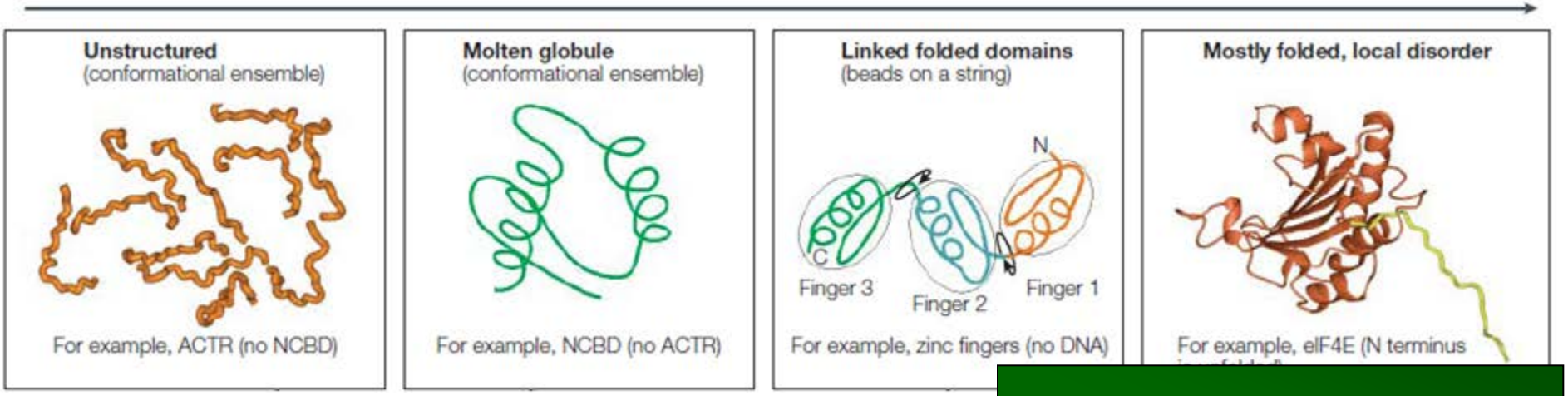
SAXS: domain spacing
WAXS: secondary structure, self assembly
DS: dynamics, persistence length
^{13}C NMR: secondary structure, self assembly, dynamics

Macrom. Rapid Comm. 2009

Unified Description of Macromolecular Structures?

Similarities between synthetic and *biological* macromolecules

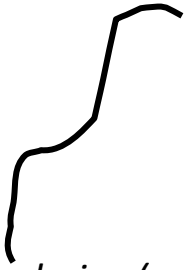
Proteins: Increasing content of "stable" 3D structure



H. J. Dyson & P. E. Wright, *Nat. Rev. Mol. Cell Biol.* **2005**, 6, 197-208

H. Staudinger: synthetic macromolecules as *models* for proteins?!

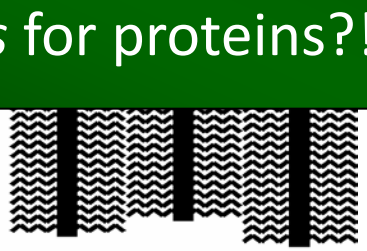
Synthetic polymers



single chains (e.g. random coil, WLC...)

networks (chemical crosslinks)

microcrystalline



bundles/crystalline polymers

D. Hinderberger, DFG-Rundgespräch, Ringberg, 2012

Why Were IDPs as a Class Recognized so Late?

Today we have the methods and know what (and that) we have to look for!

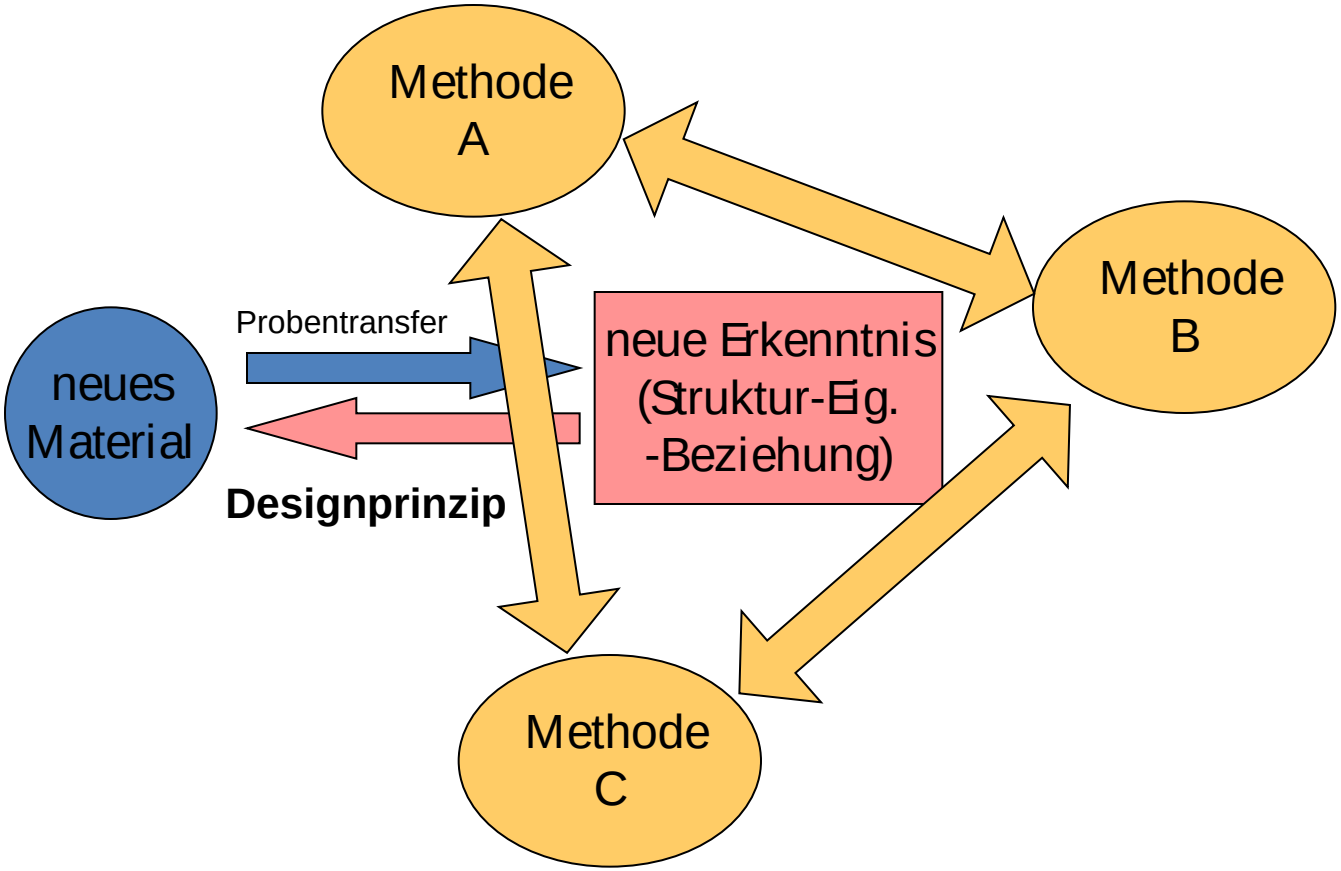
Keys for Understanding IDPs:

1. Identification of ID regions in the proteome and the genome!
   - ➢ Bioinformatics, Bioinformatics, Bioinformatics!

2. Characterization of transient structures and the whole conformational ensemble!
   - ➢ Local Methods: **NMR**, **Fluorescence**, CD, IR/Raman, **EPR**

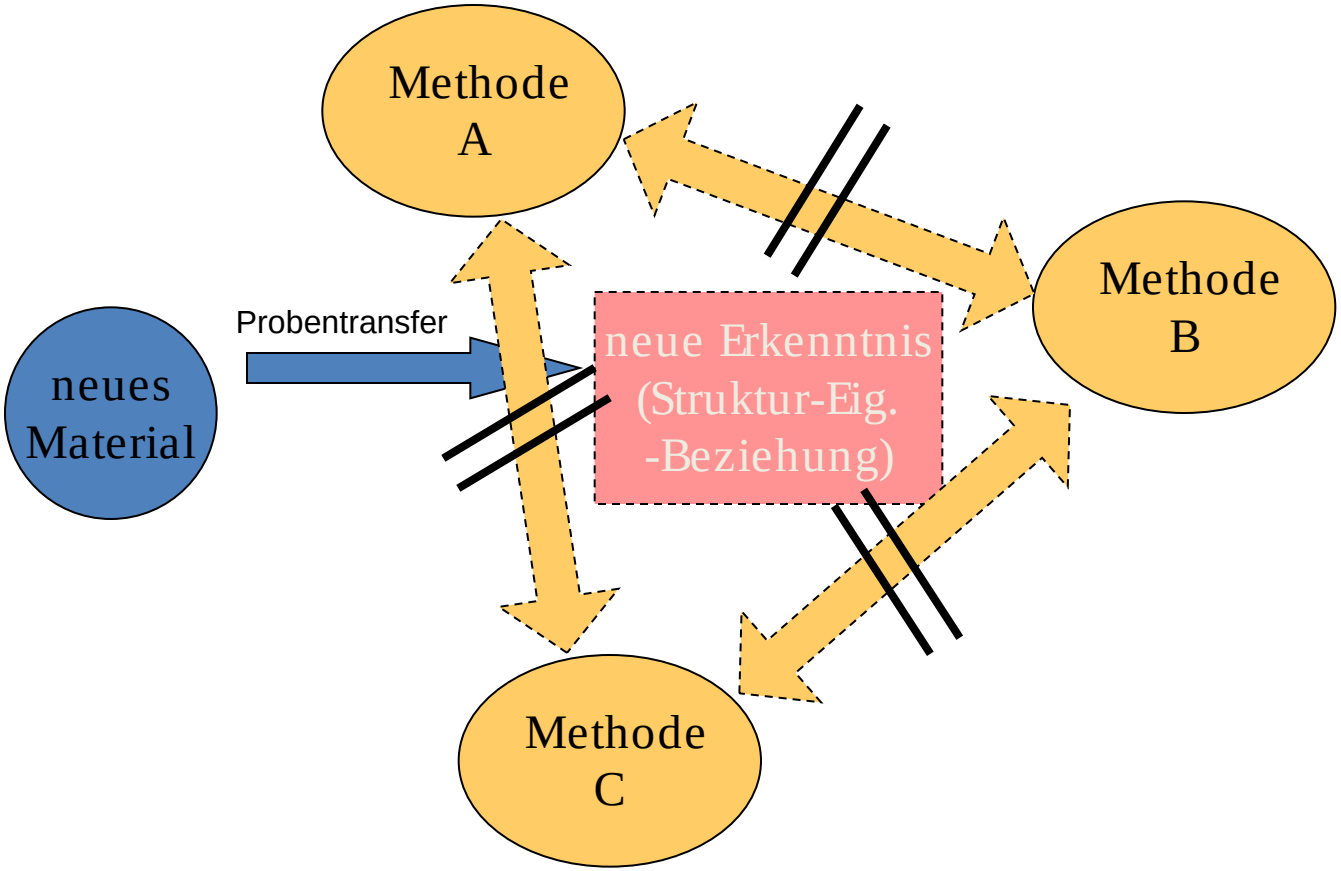
Integrierter Ansatz zur Entwicklung neuer (Polymer)Materialien

Idealfall – vs. realistische Szenarien

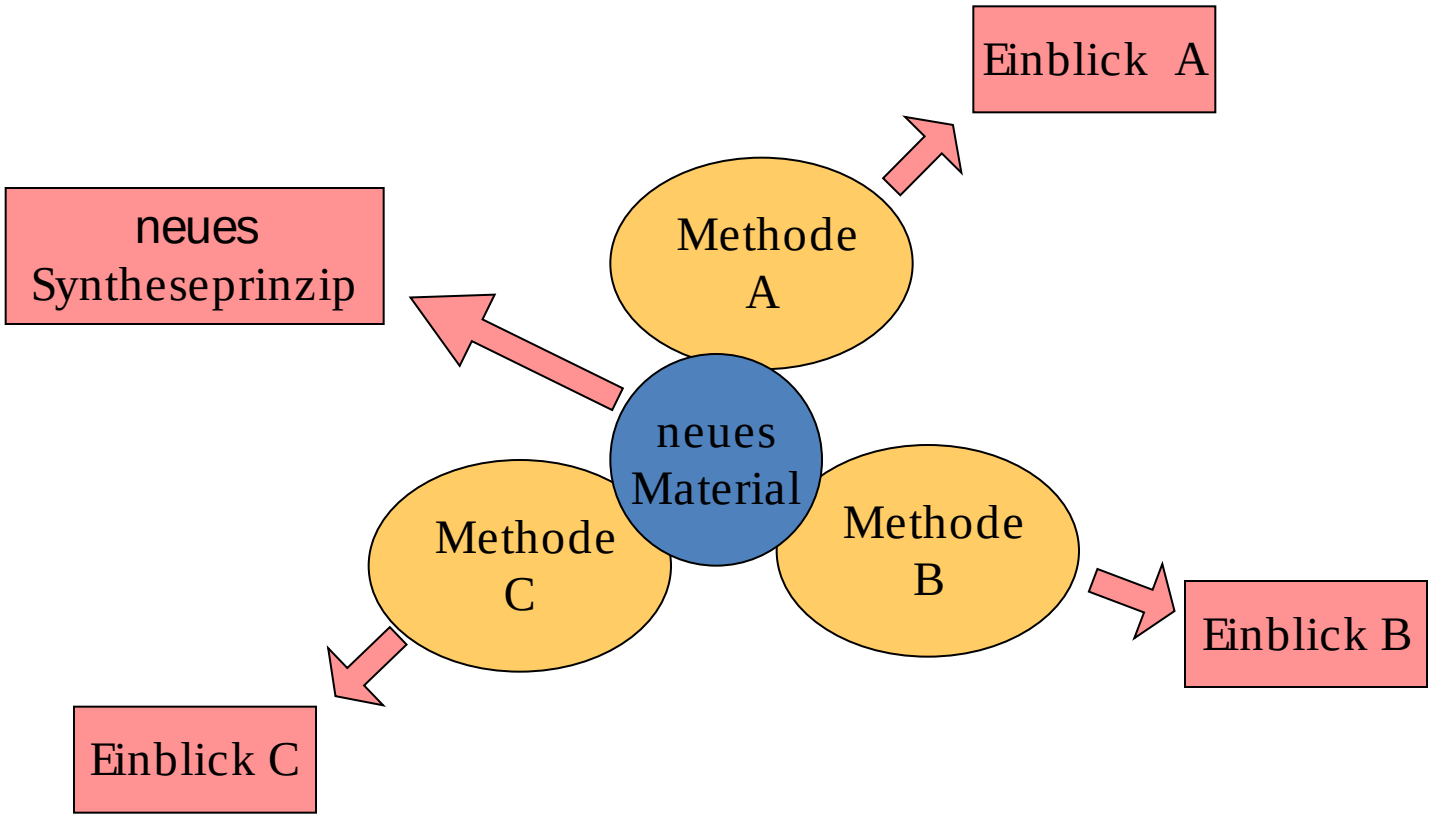


gibt es das so?
Steuerungsinstrumente?

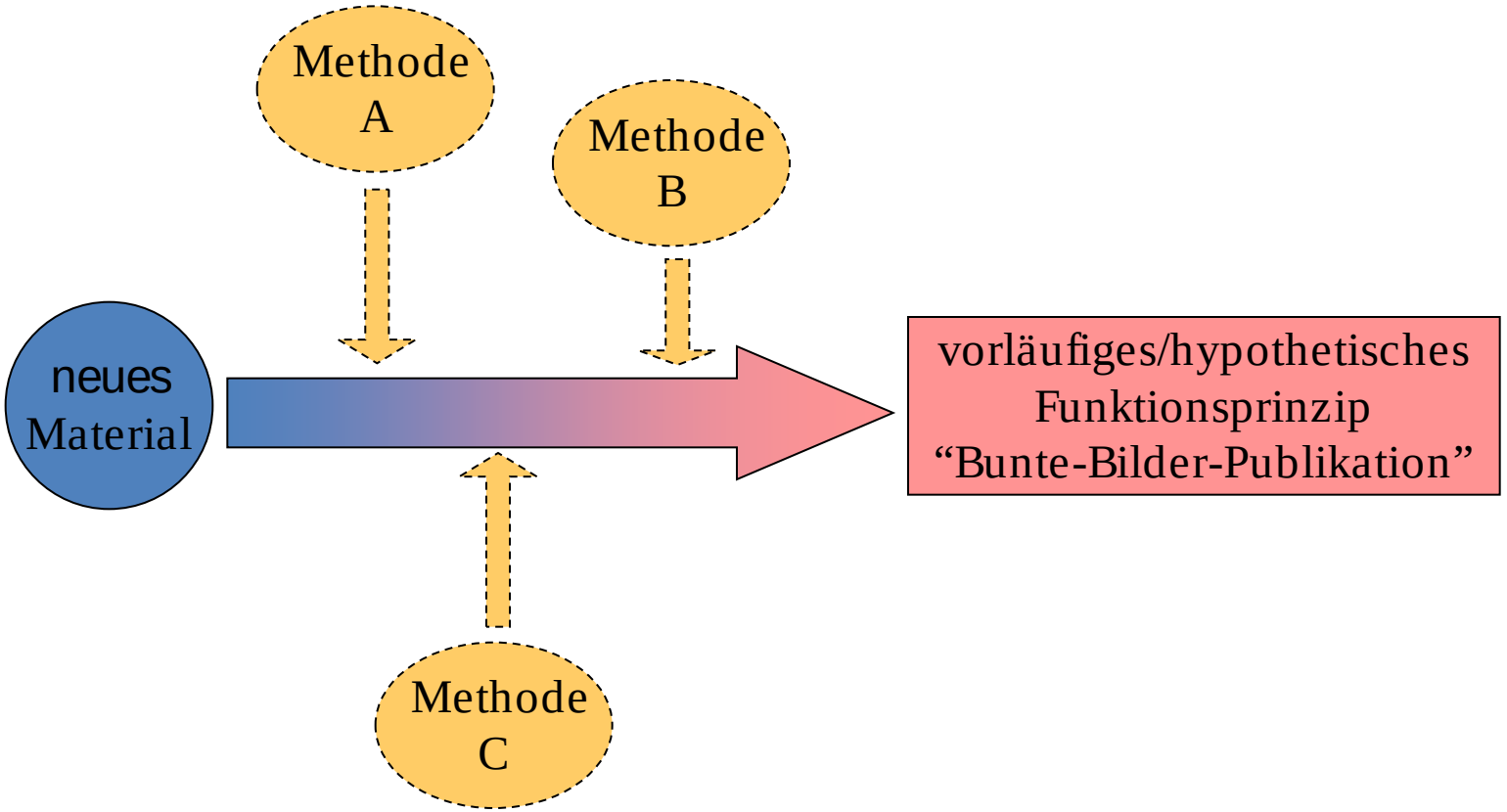
Idealfall – vs. **realistische Szenarien**



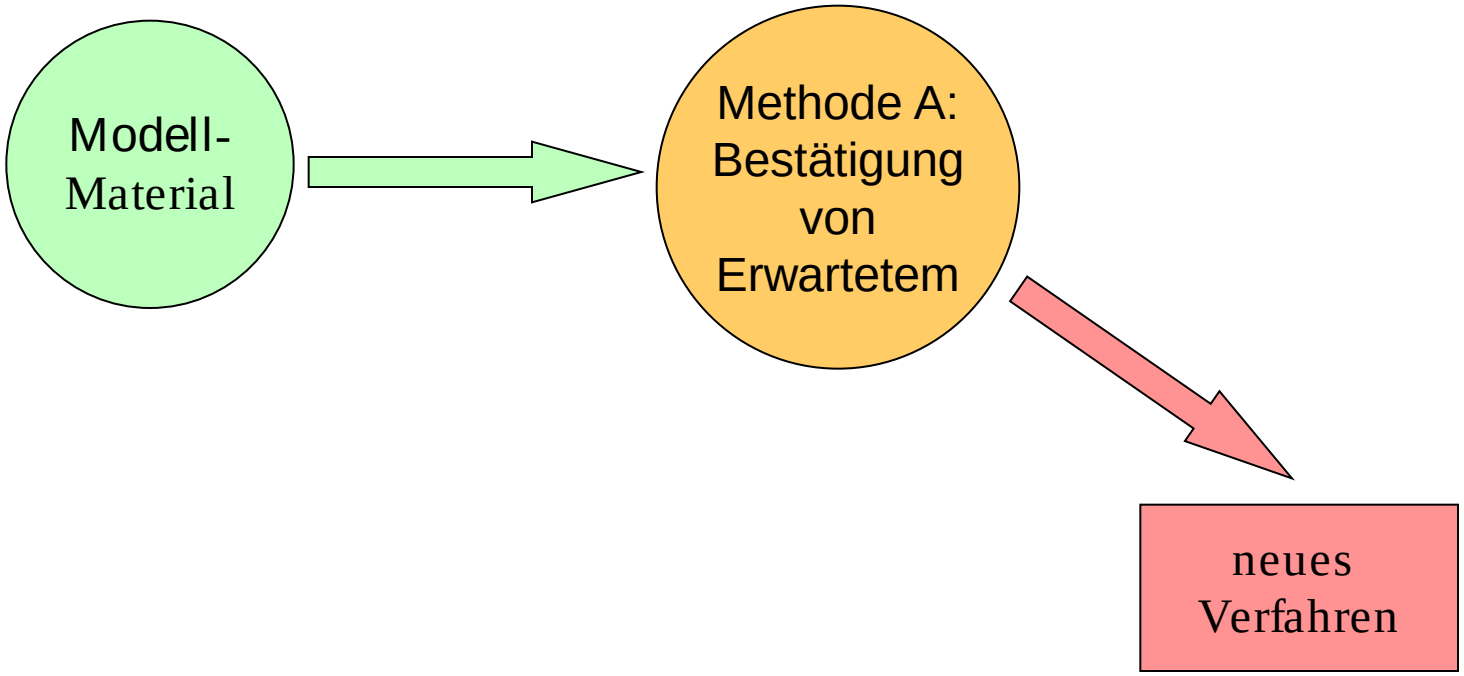
Idealfall – vs. **realistische Szenarien**



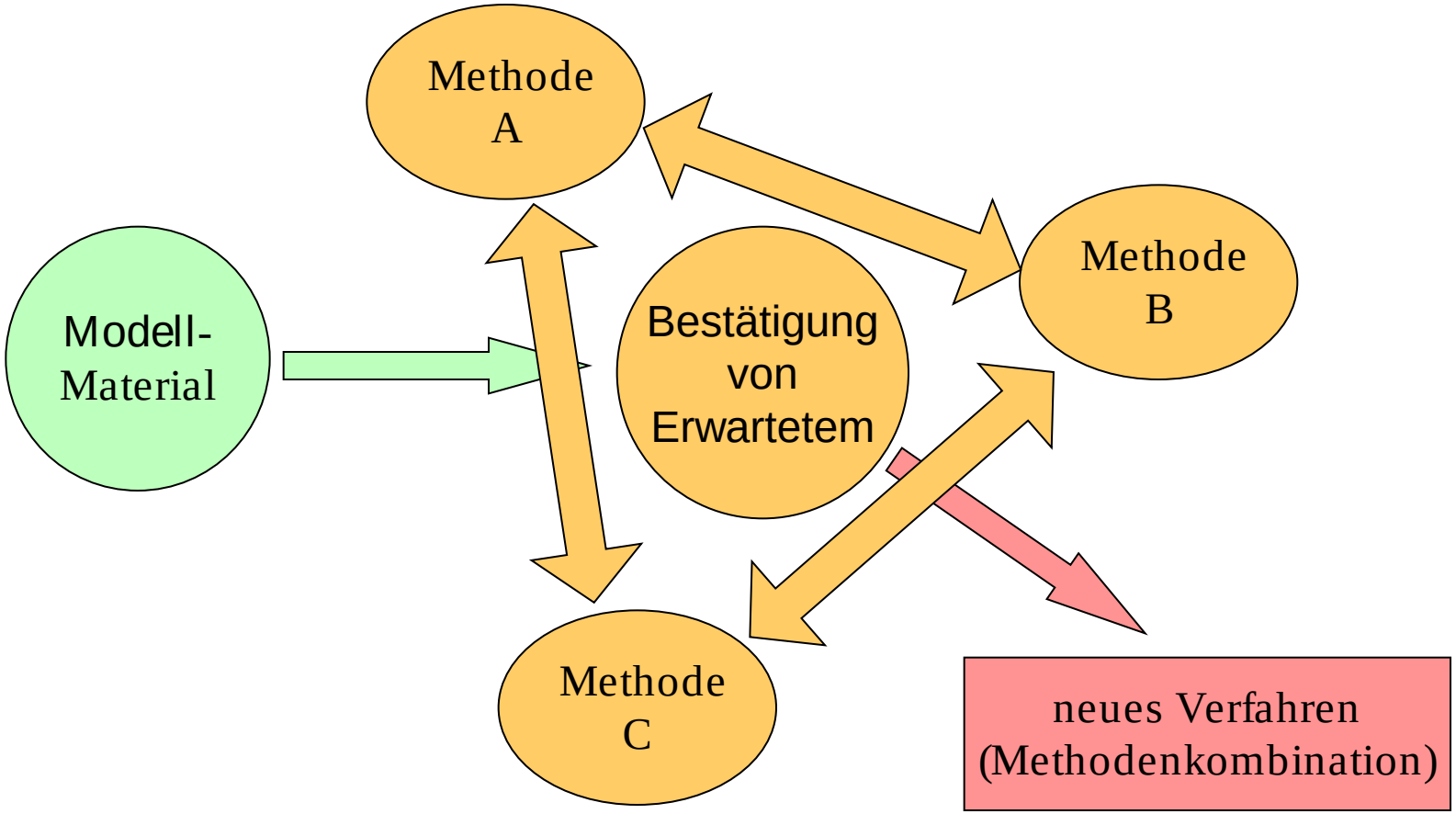
Idealfall – vs. **realistische Szenarien**



Methodenentwicklung



Methodenentwicklung



Neue Herausforderungen durch komplexe Materialien

- Inhomogenität über große Zeit- und Längenskalen
- Rolle von Unordnung und Defekten
- unerwünschte Komplexität (z.B.: “click”-links als eigenes strukturbildendes Element?)
- Rolle (teils offener) grundlegender Mechanismen (z.B. Polymerkristallisation), Notwendigkeit von Modellstudien

- oberflächliche Schlussfolgerungen durch oberflächliche Anwendung von Methoden durch nicht-Spezialisten
- Notwendigkeit der Bildung breiterer Methoden-kompetenz einzelner Wissenschafter (realistisch?) oder verbesserte Kommunikationsmodi

- Interdisziplinarität (Biowissenschaften, Halbleiterphysik…)
- Komplexität und Lösung von Teilproblemen verstellt mitunter Blick auf wirklich relevante Zieleigenschaften