What is it?

- Computational method that is used to estimate the forces between atoms within molecules and also between molecules
- **Coarse graining** - simplified molecular modeling
    - Capture system behavior using reduced representation and degrees of freedom
    - Super atoms/pseudoatoms represent a number of heavy atoms → spherical elements
    - Start withdetailed model and remove irrelevant dof→ loss of robustness?
    - Use top down approach - parameters optimized to reproduce thermophysical properties via equation of state
        - MARTINI model most efficient
            - Four-to-one mapping, i.e. on average four heavy atoms and associated hydrogens are represented by a single interaction center → 4 types of centers: polar, np, apolar, charged

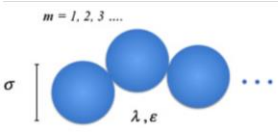

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Fig. 1. Cartoon of a SAFT CG molecule composed of m beads bonded at a characteristic distance σ. ε is the energy scale corresponding to the minimum in the intermolecular potential, while the range of the potential is determined by the repulsive exponent λ. Values for common substances are given in Table 1.

    - Two steps: mapping beads from AA scale to reduce complexity → then, define interactions
    - Bottom up approach: AA simulation to derive force fields and interactions

Why

- Reconstruction of modeled structures
- Reduce computational cost and chemical space complexity while still being accurate
- Computationally more effective and enable simulations of much longer time-scales and/or larger sizes of the systems studied
- In order to study the large size of polymer chains and the associated slow relaxation processes, a reduction of the degrees of freedom has proven absolutely necessary

Uses

- Studying protein folding mechanisms based generalized protein-like models or simulations of real proteins
- Predict protein structures

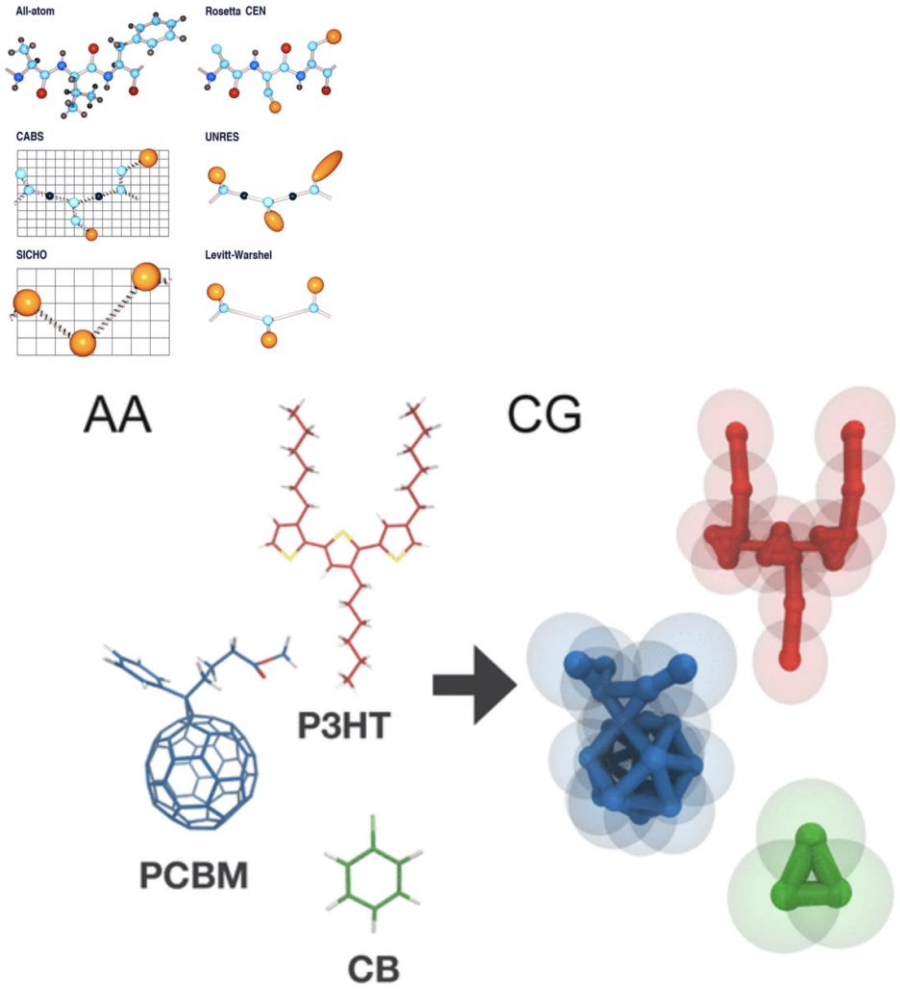

Figure 1. All-atom structures (left) and corresponding coarse-grain models (right) for P3HT (in red; a trimer is shown), PCBM (in blue), and CB (in green). The connectivity between the coarse-grain interaction sites is highlighted, while the actual size of the beads is shown with semitransparent spheres.

https://www.sciencedirect.com/science/article/pii/S0378381215300297
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