Polymorph specific RMSD local order parameters: surface melted layer thickness and polymorph selection
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Structural order parameters

- Crystal nucleation and growth involves structural changes that are often described by order parameters. Order parameters differentiate between structures.
- Computing polymorphism is important in pharmaceutical sciences.
- Controlling polymorphism is important in pharmaceutical crystallization. Mechanistic studies of polymorph selection require coordinates which can distinguish polymorphs.

Template based RMSD OP

- Compare a set of templates of the known polymorphs to the local environment of each molecule in the simulation.
- Use the Kabsch algorithm to find the rotation that minimizes RMSD between the template and the local environment.
- The RMSD value for each polymorph template is the local polymorph specific order parameter value.

Glycine template matching

- Use the matching algorithm to compare the local environment of each glycine molecule to templates for each glycine molecule in the unit cell of each polymorph.
- The lowest RMSD score among templates for all polymorphs is the polymorph specific order parameter value.

Surface melted layer of solvated nuclei

- Steinhardt order parameters, as extended by Frenkel and coworkers, can differentiate liquid from solid for studies of crystal nucleation in simple liquids, proteins, and colloids.
- Recently local averaging of these order parameters was used to differentiate the BCC, FCC, and HCP polymorphs in a Lennard-Jones fluid.

Inter molecular coordinates

- More general frameworks for order parameters have been developed for complex systems utilizing inter and intra molecular coordinates, and combinations of spherical harmonic order parameters.

Matching algorithm

- RMSD based order parameters require an atom by atom correspondence. Comparing all possible combinations of atoms is computationally expensive.
- We resolve this problem through molecular pruning and two stage matching procedures.

Glycine crystal structure

- Glycine forms a zwitterion in solution and in the crystal structures.
- Glycine forms three polymorphs at ambient conditions.
- γ-glycine forms first out of aqueous solution.

RMSD based OP for bulk crystal

- For glycine we remove hydrogen atoms since they contribute little important structural information.
- The π rotational symmetry of the CO 2 group of glycine is removed with a dummy atom which replaces the two oxygens in a way that loses essentially no conformational information.

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References