Nucleation of molecular crystals

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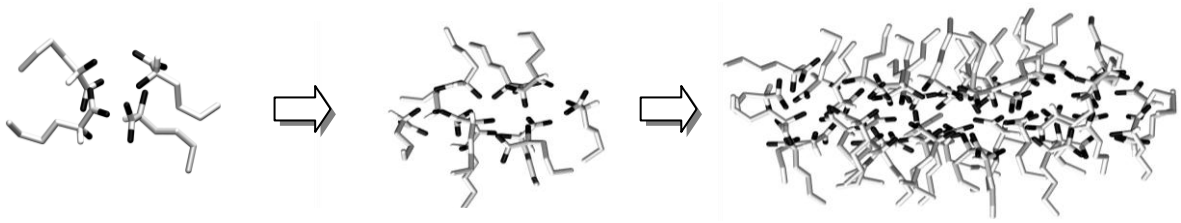

4 molecules *10 molecules* *50 molecules*

We investigate the early stages of molecular crystal nucleation by means of a combined Monte-Carlo/molecular dynamics simulation approach. Along this line, the time scales for solute migration to the aggregate are efficiently bridged, whilst detailed simulated annealing is applied to aggregate relaxation.

Starting from a dimer, the Kawska-Zahn method allows the investigation of the mechanisms of molecule-by-molecule association, the formation of pre-nucleation clusters, nucleation and aggregate growth [1].

Here, we demonstrate this approach for two molecular species, i.e. D/L - norleucine and benzamide. While the polymorphism of the former has been thoroughly explored by Anwar et al [2], dispersion-corrected density functional calculations are used to rationalize the subtile energy differences in the most important polymorph structures of benzamide.

On the basis of this in-depth understanding we suggest nucleation scenarios as guide to synthesis [3,4,5].

The pictures illustrate the early stages of D/L - norleucine molecule association (left) and the transition (middle) to later stages of aggregate growth with reflect the formation of layered structures (right).

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