Nucleation of molecular crystals

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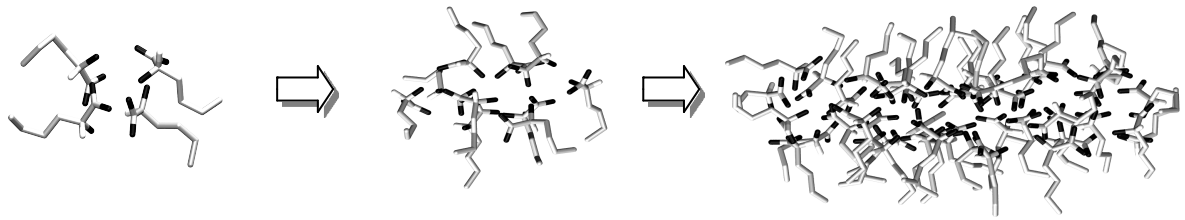

4 molecules *10 molecules* *50 molecules*

We investigate the early stages of molecular crystal nucleation by means of the Kawska-Zahn approach [1]. Along this line, molecular association, the formation of pre-nucleation clusters, nucleation and aggregate growth is explored.

Currently, our focus is set to two systems, i.e. D/L - norleucine using the excellent force field of Anwar et al [2] and benzamide for which we are developing a force field of similar accuracy.

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).

[1] A.Kawska, J.Brickmann, R.Kniep, O.Hochrein, D.Zahn, J. Chem. Phys., 124 (2006) 24513.
[2] Sigrid C. Tuble, Jamshed Anwar, and Julian D. Gale , J. Am. Chem. Soc. , 2004, 126, 396 - 405