98st MSS-Seminar
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Nägelsbachstr. 49b

Complex crystal structures from computational self-assembly

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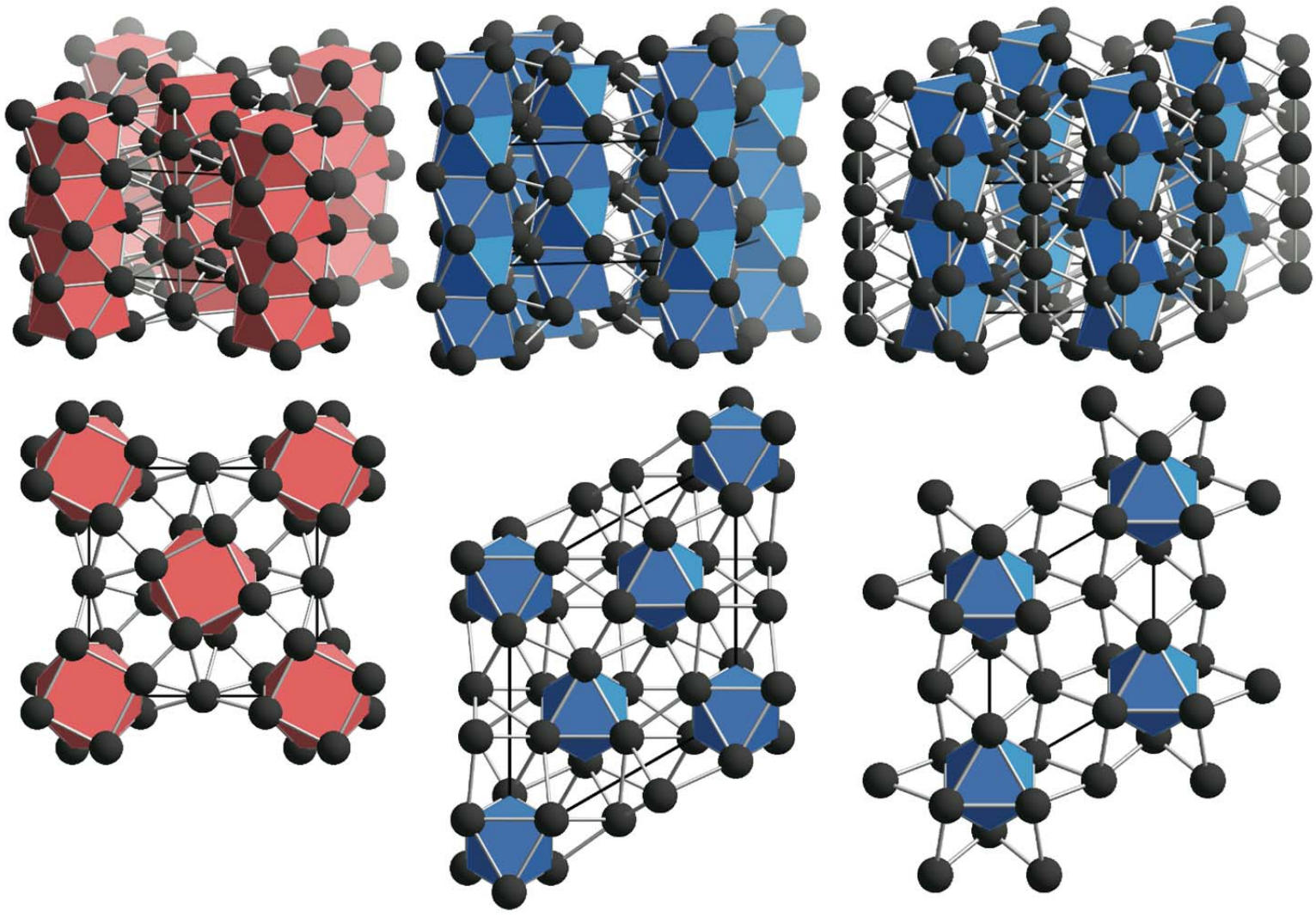

On the atomic scale, complex structures have been known to exist for decades and their origin, *e.g.*, in intermetallic systems, has yet to be explained [1]. Soft matter systems have so far mostly been found to exhibit simple structures, but with an increasingly versatile toolbox for creating various building blocks and interactions, the number of non-trivial geometries has recently started to grow (e.g., [2]). We aim to understand when and how complex structures – on multiple length scales – form, by studying the self-assembly and phase behavior of particles with tunable, isotropic pair potentials. Using the highly parallel molecular dynamics code HOOMD-blue [3], we simulate a wide range of one-component systems and observe the resulting phases. We report a rich variety of crystal structures, ranging from the well-known sphere packings and other simple structure types, to giant-unit cell structures and quasicrystals [4]. By exploring the crystal structures and structure formation behavior of these simple model systems, we aim at describing and understanding diverse experimental systems on the atom and soft matter length scales under the same terms.

[1] J. Dshemuchadse, D. Y. Jung, W. Steurer, Acta Crystallogr. B 67, 269–92 (2011).
[2] S. Chanpuriya, K. Kim, J. Zhang, S. Lee, A. Arora, K. D. Dorfman, K. T. Delaney, G. H. Fredrickson, F. S. Bates, ACS Nano 10, 4961–4972 (2016).
[3] J. A. Anderson, S. C. Glotzer, http://arXiv.org/abs/1308.5587 (2013). http://glotzerlab.engin.umich.edu/hoomd-blue/
[4] M. Engel, P. F. Damasceno, C. L. Phillips, S. C. Glotzer, Nature Mater. 14, 109–116 (2015)