Master's thesis and/or Ph.D. thesis opening

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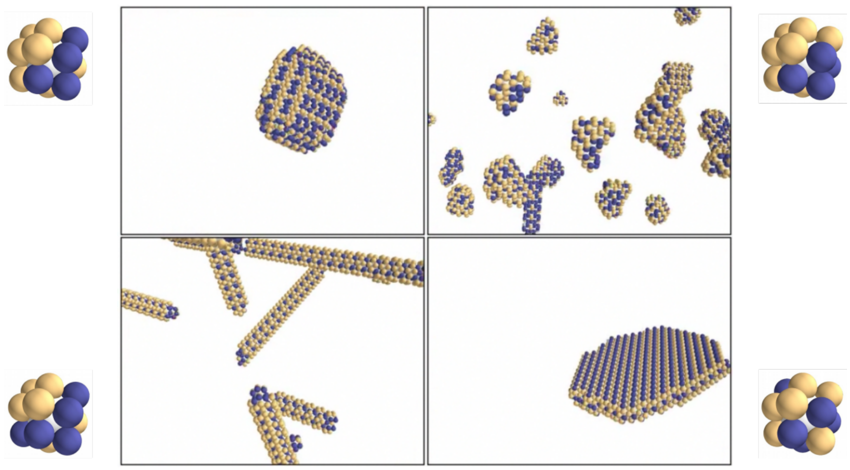
Renormalization group analysis of frustrated self-assembly

(theoretical thesis: mostly analytics, some numerics)

Self-organization is key to the function of living cells – but sometimes goes wrong! In Alzheimer's and many other diseases, normally soluble proteins thus clump up into pathological fiber-like aggregates. While biologists typically explain this on the grounds of detailed molecular interactions, we have started proving that such fibers are actually expected from very general physical principles. We thus show that **geometrical frustration builds up when mismatched objects self-assemble, and leads to non-trivial aggregate morphologies, including fibers.**

While our current numerical simulations let us monitor the aggregate formed by copies of a given irregular particle, we do not yet understand its dimensionality from first principles. Here we will **tackle this problem using ideas inspired by the renormalization group**. We will thus represent the shape of the particle as an orientation-dependent coupling matrix between two neighbors. By repeatedly applying a decimation procedure *à la* Kadanoff to the system, we will drastically reduce the enormous space of all possible coupling matrices to a few fixed points corresponding to finite clusters, fibers, sheets and crystals. An internship will start with a transfer matrix calculation applying this procedure to a 1D system. A PhD will involve some non-trivial 3D discrete geometry and will likely require delving into some linear algebra to understand the properties of our matrix universality classes.

Beyond protein aggregation, this project opens investigations into a **new class of "disordered" systems where the disorder is carried by each identical particle** instead of sprinkled throughout the system, and will help define the much-debated notion of **frustration in dilute systems**. This collaboration with Pierre Ronceray (Princeton U.) will ideally lead to collaborations with the experimental groups of Seth Fraden (Brandeis U.) and Friedrich Simmel (T.U. Munich).



In our simulations, complex lattice particles with geometrically incompatible orientational preferences (*in the corners: sites with identical colors attract*) give rise to aggregates of different dimensionalities.