**Title**: TBD

**Intro/general motivation**:

* **Reconfigurable systems** hold great promise for enabling adaptive material applications such as next-generation self-healing materials, wet computing information storage, and responsive photonic devices
  + Existing examples of reconfigurable materials are limited to macroscale systems for printed or otherwise manually arranged particles
  + However, such methods are infeasible at the nanoscopic scales required for realization of the aforementioned applications
* **Equilibrium self-assembly** can be used to nanofabricate ordered structures by allowing atoms, molecules, or colloidal particles to sample many potential configurations through thermal fluctuations
  + The resulting self-assembled structure is the configuration that minimizes the free energy
  + In equilibrium systems, colloidal-scale self-assembly is a well-characterized process
  + Particle anisotropy, specifically shape, has been shown to determine the structure of self-assembled colloidal crystals, even in the absence of explicit inter-particle interactions
* **Experimentally**, many **synthetic colloidal systems** do no assemble reliably or robustly
* In contrast, **biologically assembled materials** often reliably assemble into metastable, non-equilibrium states that allow them to rapidly respond to external stimuli structurally and functionally
  + Many of these biological structures are stabilized by the constant input of energy from ATP, which provides the driving force for non-equilibrium self-assembly in these systems
* This robust self-assembly inspires engineers looking to design synthetic nanofabrication processes
  + However, the fundamental physics of such driven non-equilibrium self-assembly remains poorly understood
* By understanding the principles governing driven non-equilibrium self-assembly, we can eventually design pathways to robustly self-assembly reconfigurable, adaptive materials for nanoscale applications

**Background**:

* “Active matter” describes driven non-equilibrium systems in which a self-propulsive driving force is applied to each particle
  + These systems display a wealth of non-equilibrium behavior, such as a collective motion (e.g. swarming) and giant density fluctuations (e.g. clustering)
* Experimental and theoretical active matter research has focused primarily on the behavior and self-assembly of isotropic particles
  + While useful for defining the basic physics of these systems, such particles do not have a natural “alignment rule” allowing for torques to be effected on neighboring particles
  + However, anisotropic particles with shape *are* able to alter the orientations of neighboring particles, and we know that particle shape alone is sufficient to direct self-assembly in equilibrium systems
* Thus, a natural question arises: how does particle anisotropy, specifically shape, impact self-assembly in drive non-equilibrium systems?

**Proposed work**: **How does particle anisotropy, specifically shape, impact self-assembly in driven non-equilibrium systems?**

* Computational capabilities allow the study of active systems on large enough time and length scales to be predictive
* Further, experimentally determining the key drivers of self-assembly is prohibitively time-consuming
* By computationally developing an understanding of the drivers of non-equilibrium self-assembly, I will guide experimental tests towards systems of interest

**Aim #1**: **Predict structures and formation kinetics of self-assembled anisotropic hard particle systems**

a) (each of these should basically be what you’ll do to get a figure)

b)

c)

**Hypothesis and rationale for it**: Self-assembled structures in driven systems can be related to the system density, applied driving force, and anisotropy of the particles

**Key preliminary results**: (TBD from what I’m working on now and can get done in the next few weeks)

**Experimental design/specific methods**: Active particles will be modeled using HOOMD-blue molecular dynamics, and open source software package built to run in parallel on GPUs and CPUs, and developed and maintained by the Glotzer lab. Anisotropic shape interactions are accounted for with a discrete element method, borrowed from the granular matter community (?) and implemented in HOOMD-blue. The onset, structure, and kinetics of clusters of active particles will be evaluated over varying driving forces and system density.

*Analysis*: Clusters of active particles have previously been shown to assemble into “active crystals”. The emergence of clusters versus driving force and density can be compared with the sparse literature on anisotropic active particles, while structure can be checked against known equilibrium assemblies. Equilibrium self-assembly of anisotropic particles can be validated using hard-particle Monte Carlo in HOOMD-blue, by equating active driving force to system pressure.

**Complications/alternative strategies**: These Brownian simulations take a long time to run; force.active is currently not MPI compatible; maybe do them in NVT, could be easier to calculate?

**Aim #2**: **Evaluate material reconfigurability as a means of tailoring nanofabrication and information storage for nanoscale applications**

a)

b)

c)

**Hypothesis and rationale for it**: If non-equilibrium self-assembly of active particles is dependent upon their anisotropy and driving force (Aim #1), then reconfiguring the particle’s shape and driving force should allow the active crystal structure to transition to a new steady state structure.

*Importance*: If reconfigurabilty in non-equilibrium allows us to reach otherwise inaccessible structures, this would be of further interest as a nanofabrication approach. Additionally, reconfigurability-induced switching of a material’s structure could be explored as a way of storing information (“memory”) in a material. Such work could be extended as a potential solution for wet computing information storage.

**Key preliminary results**: N/A, maybe come up with something if time…

**Experimental design/specific methods**: All simulation can be carried out as in Aim #1, with particle shape or driving force reconfiguration attempted after system is at steady state.

*Analysis*: From Aim #1, we will already know the expected crystal structure of a set of anisotropic shapes with which these results can be compared.

**Complications/alternative strategies**:

**Aim #3**: **Evaluate the impact of hydrodynamics on active anisotropic self-assembly, in preparation for experimentally realizing self-assembly of active anisotropic particles**

a)

b)

c)

**Hypothesis and rationale for it**: Incorporating hydrodynamic forces will affect the active crystal kinetics of formation, but not the structure formed

**Key preliminary results**: N/A

**Experimental design/specific methods**: Hydrodynamic effects are neglected in Aims #1 and #2 to isolate the effect of particle anisotropy on self-assembly. They can be approximated by the inclusion of small “solvent” particles using HOOMD-blue.

*Analysis*: The assembly diagrams from Aim #1 can be replicated, with the inclusion of hydrodynamics. These results can be verified experimentally as proof of concept for designed non-equilibrium self-assembly.

**Complications/alternative strategies**:

**Timetable:**

Like, a year should be enough time, right?