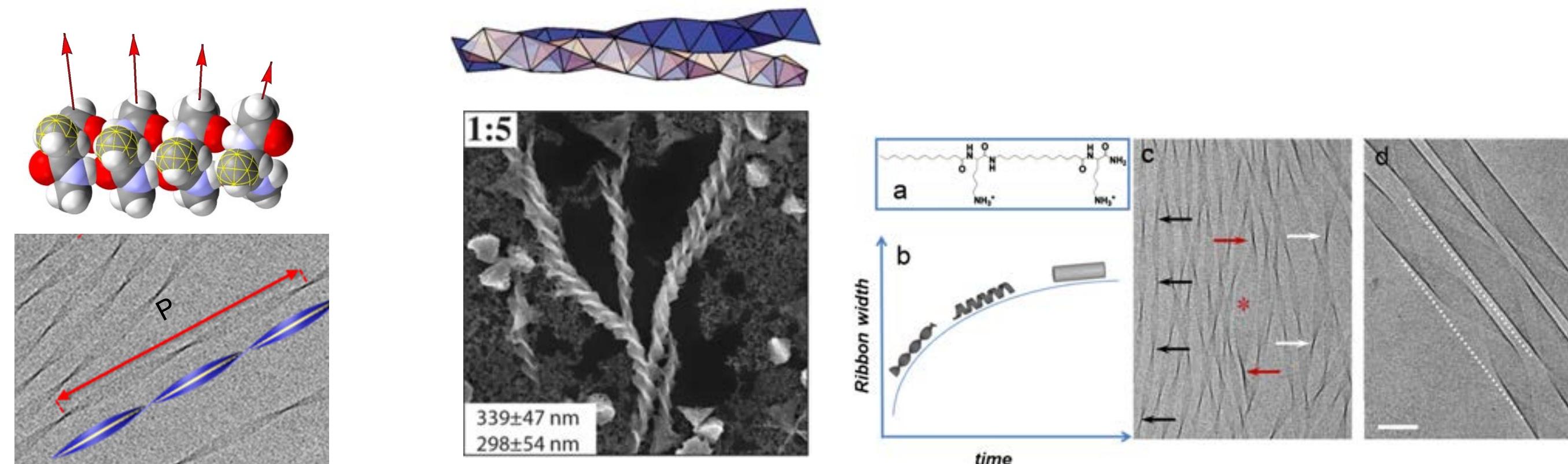


- IRG-1 aims to design self-assembly with well-defined dimensions much larger than the building blocks
- We develop a new coarse-grained model to connect particle design to self-limitation and escape behaviors
- We connect continuum theory of frustrated assembly to features of discrete particles and their interactions

Self-limiting ribbons and escape in amphiphile and nanoparticle assembly



Zhang *Nat. Com.* (2019)

Serafini *Nat. Com.* (2021)

Ziserman, PRL (2011)

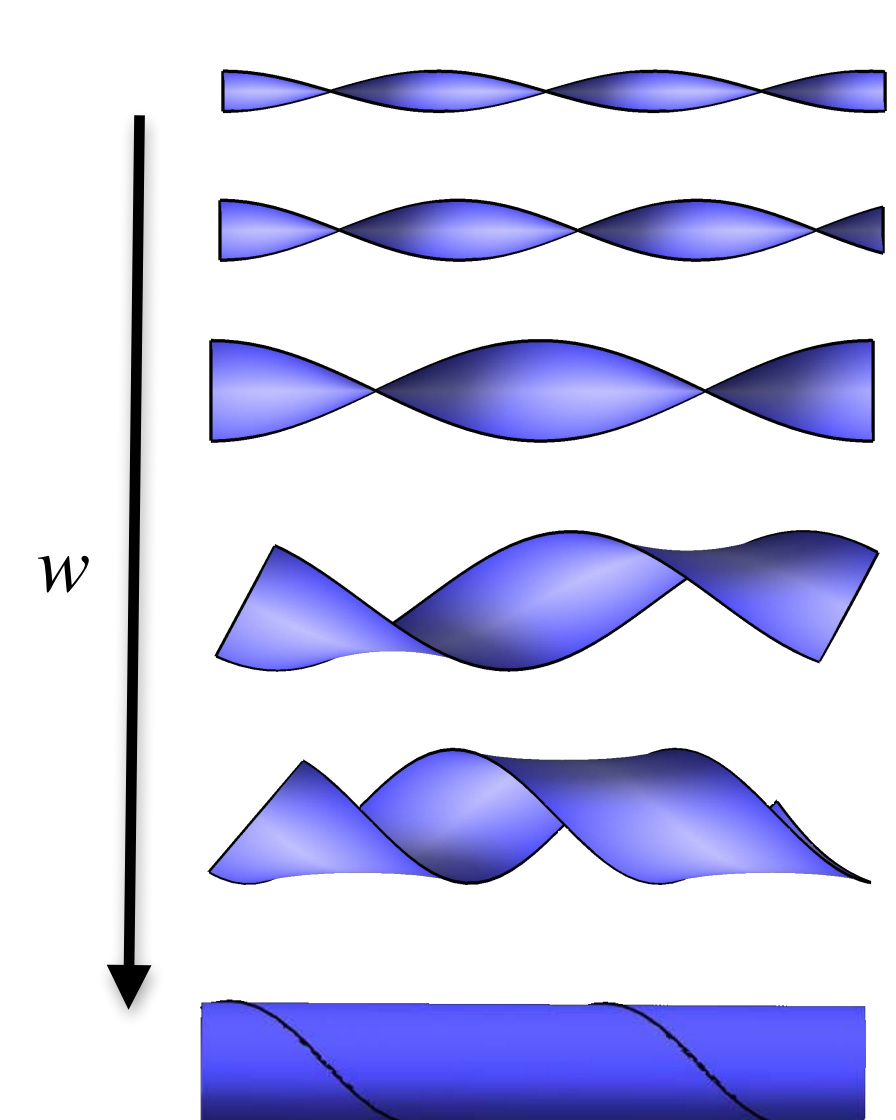
How can we design particles to extend self-limiting assembly size?

Theory of frustrated ribbon morphologies and escape to tubules by flattening

Continuum ribbon elastic energy + line tension: $F = E + 2\Lambda L$

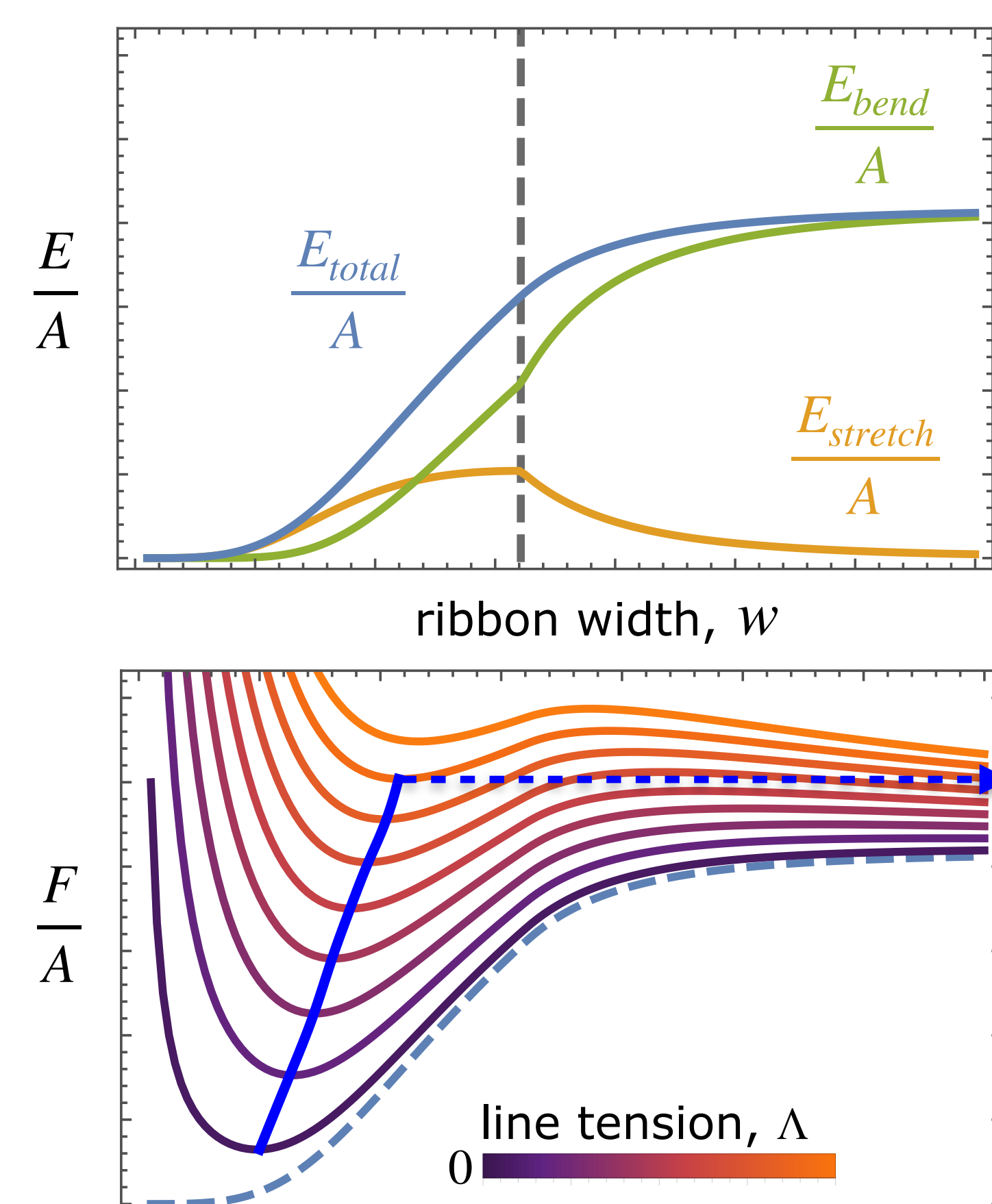
ribbon shape (self limiting)

$$E_{narrow} \sim Yw^5\kappa_0^4L$$

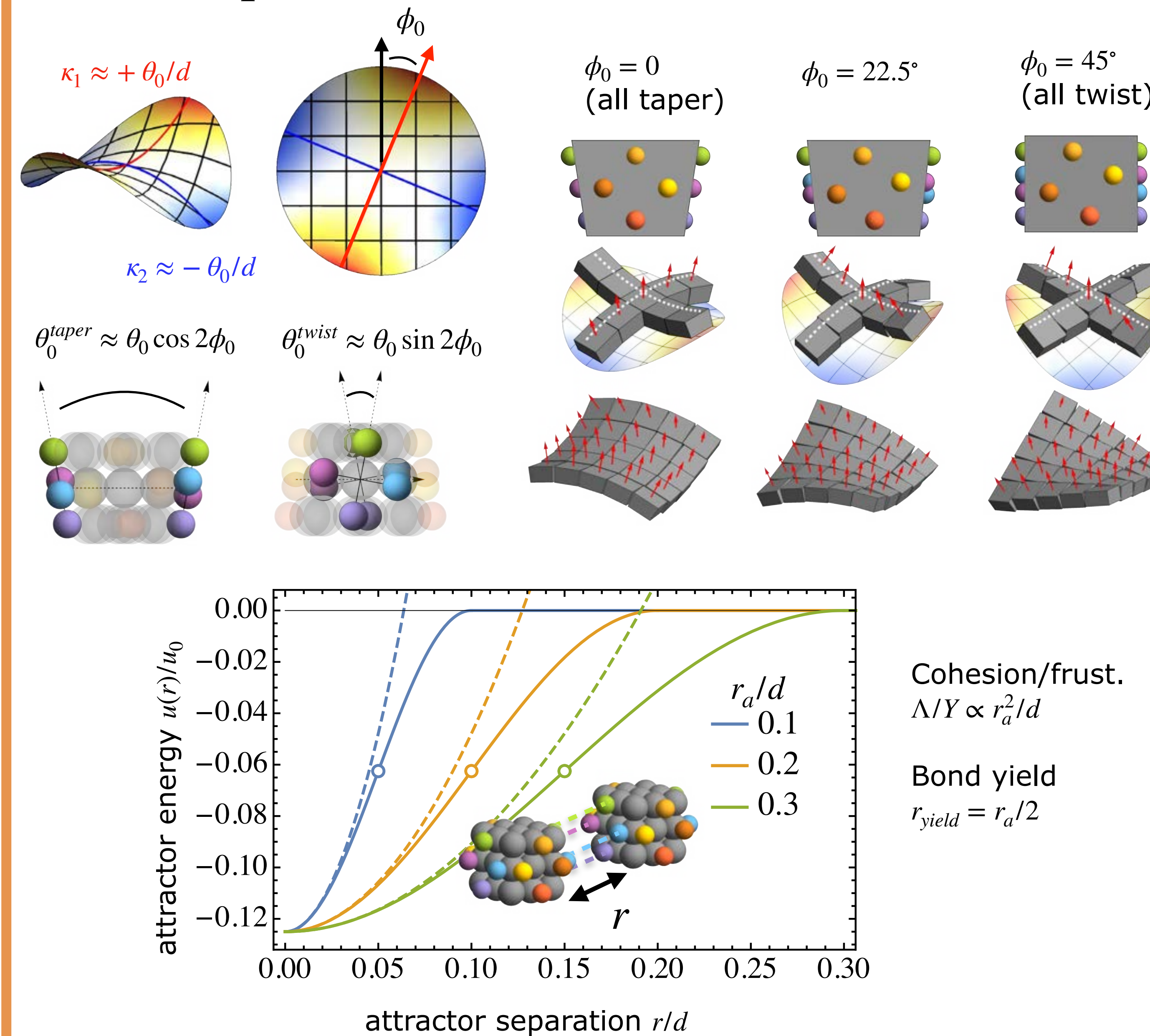


cylindrical shape (flat)

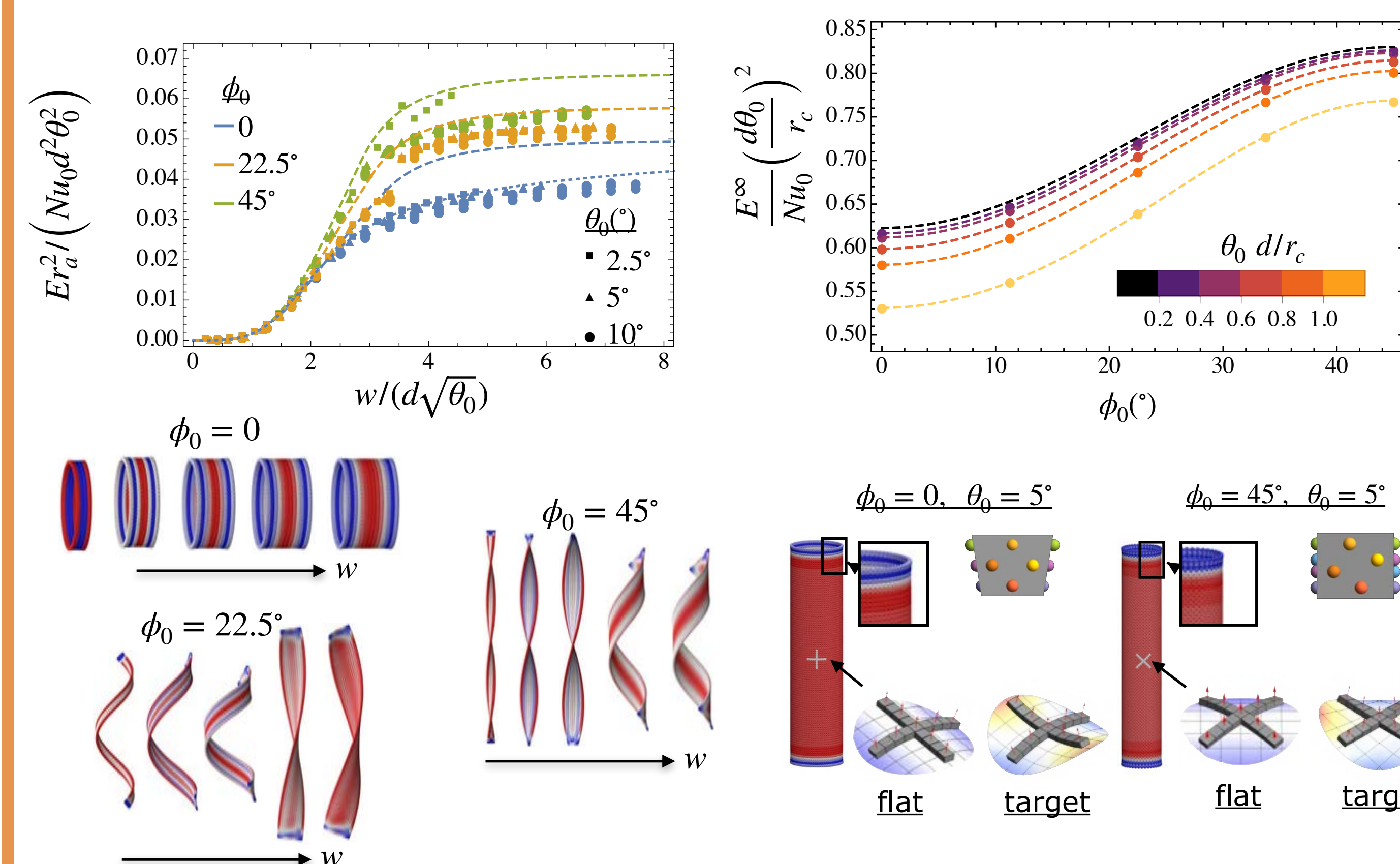
$$E_{flat}/A = B\kappa_0^2$$



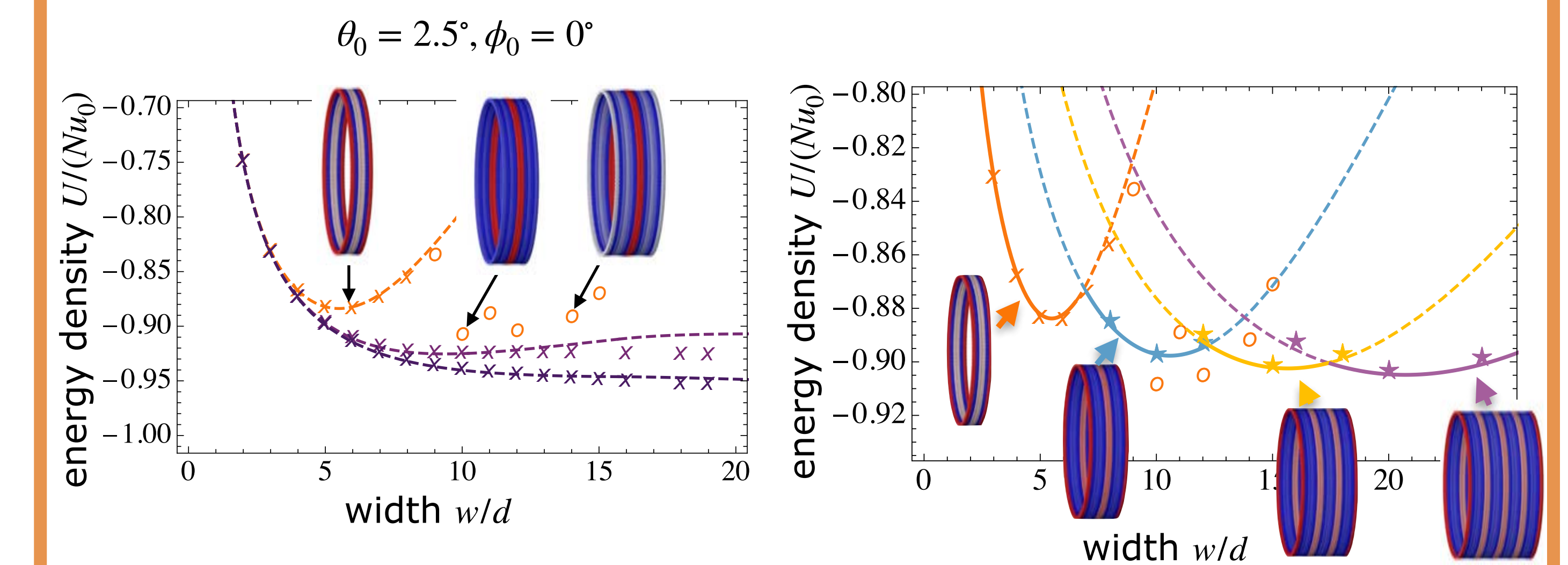
Discrete particle model with tunable frustration



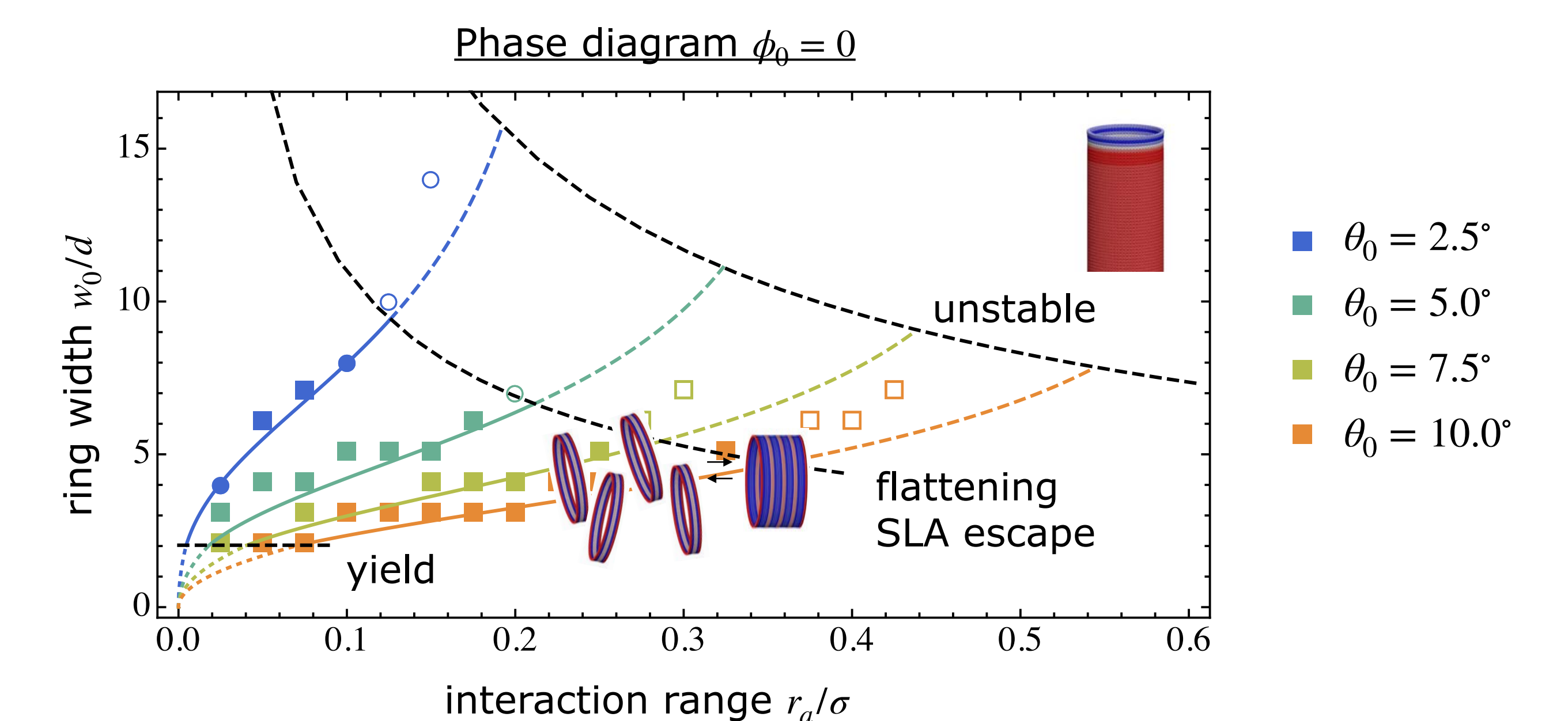
Role of bending stiffness anisotropy and strain softening in escape by flattening



Yielded bonds allow hierarchical assembly and imply lower limit to frustration-limited assembly



* Inter-ring binding, $\gamma_{stack} \approx 0.15u_0$ per bonded pair of particles



- Upper limit to self-limiting assembly sizes connected to particle geometry, distinct bending modes, and range of interaction
- Self-limiting structure may form hierarchical assembly
- Lower size limit from the interaction range, limit to strain that can be supported in assembly before yield

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