Accelerated Self-Replication under Non-Equilibrium Periodic Energy Delivery

Rui Zhang, David A. Walker, Bartosz A. Grzybowski, and Monica Olvera de la Cruz

From DNA to cells to organisms, self-replication is a carefully orchestrated process spanning multiple length scales and ensuring the sustainability of life on Earth. One key, but often overlooked, characteristic of self-replication systems is the need for energy "cycling" to bind/unbind the system's components. During self-replication, the monomers have to first assemble onto the template (where they bind to one another), but then must disengage from this template to serve as templates themselves.

In this study, we ask whether the overall efficiency of self-replication (measured by the rate at which templates are replicated) can be controlled and optimized by the frequency at which energy is supplied to the system. In our model (inspired by a recently-demonstrated class of colloids), particle dimers replicate from particle monomers with the interactions between all of these species toggled between attractive and repulsive by external pulses of (light) energy (Figure 1).

We find that the rate of self-replication does not require constant energy expenditure, but is heavily influenced by the timing of the energy delivery and that periodic energy delivery can increase the rate of self-replication.

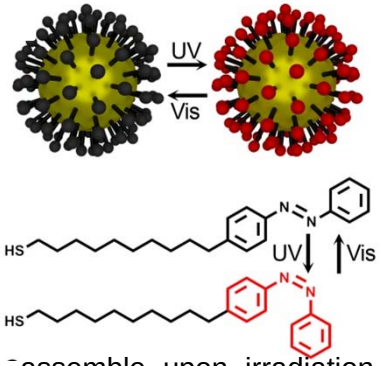
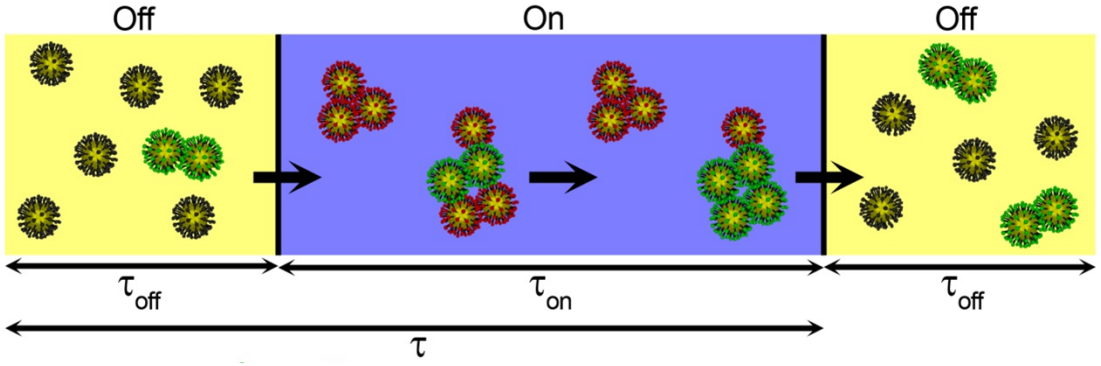


Figure 1. Our system is inspired by the experiments with photoswitchable Au NPs covered with azobenzene-terminated thiols. Such systems have been shown to assemble upon irradiation with UV light (ON state) when the azobenzenes develop dipole moments and can interact via attractive dipole-dipole interactions. In the absence of UV irradiation (OFF state), azobenzenes re-isomerize into the zero-dipole *trans* form.



Scheme of a self-replicating system driven by time-varying energy inputs.
Template dimers (shown in green) have the ability to bind monomers (shown in red) and cross-link them to form daughter templates. The periodic light/energy input **τ**

We thank Prateek Jha and Vladimir Kuzovkov for stimulating discussions during development of the model. Numerical simulations were performed using the Northwestern University High Performance Computing Cluster Quest. This work was supported by the Non-Equilibrium Energy Research Center (NERC), which is an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0000989. DAW thanks the fellowship from the Northwestern University Materials Research Science and Engineering Center (NUMRSEC) funded by the NSF under Award Number DMR-1121262.