Inverse Design of Equilibrium Cluster Fluids
RYAN JADRICH, JONATHAN BOLLINGER, BETH LINDQUIST, THOMAS TRUSKETT, University of Texas at Austin — Equilibrium cluster fluids have garnered much recent attention, but the types of interparticle forces that can lead to self-assembly of such entities have not been systematically explored. As a step towards addressing this, we leverage powerful inverse design tools to fabricate a fluid of monodisperse, spherical, liquid-droplet-like clusters of a desired size and good center of mass mobility. The inverse designed pair potential possesses a broad attractive well and narrow repulsive barrier at larger separations—a qualitatively different form as compared to the so-called SALR potential [short-range attractive (SA) and long-range repulsive (LR)] often associated with equilibrium cluster formation in colloids. Such differences suggest alternative mechanisms for cluster formation leading to structured fluids with qualitatively different static and dynamic properties. Lastly, we explore the representability of our inverse designed potentials through simple parametrized forms.