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Designing thermo-responsive nanocomposites with anti-fouling properties YA LIU, GERALD MCFARLIN, University of Pittsburgh, XIN YONG, Binghamton University, OLGA KUKSENOK, ANNA BALAZS, University of Pittsburgh — Inspired by marine organisms that utilize active "defense" (such as active cilia) to prevent the biofouling of their surfaces, we use computational modeling to design synthetic gel-based composite films that provide dual "defense" for antifouling applications. We design a nanocomposite gel film that can be harnessed to repel a variety of particles via either a temperature change or an imposed shear. Incorporation of stiff hydrophobic posts into a gel composed of cross-linked poly(N-isoproylacrylamide) chains allows us to drastically alter the film's surface properties when gel undergoes temperature-induced volume phase transition. Depending on whether the system's temperature is below or above the lower critical solution temperature (LCST) of the gel, the posts are hidden in the swollen gel or exposed to the external solution. We model our system using dissipative particle dynamics (DPD); we validate our model through comparisons with Flory-Rehner theory. We focus on the influence of shear and temperature on the position of the particle in the system and isolate the conditions under which adsorption of particles of different sizes to the substrate is effectively prevented.

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