

Abstract Submitted  
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**Amphiphilic gold nanoparticles as modulators of lipid membrane fusion**<sup>1</sup> MUKARRAM TAHIR, ALFREDO ALEXANDER-KATZ, Massachusetts Inst of Tech-MIT — The fusion of lipid membranes is central to biological functions like inter-cellular transport and signaling and is coordinated by proteins of the soluble N-ethylmaleimide-sensitive factor attachment protein receptors (SNAREs) superfamily. We utilize molecular dynamics simulations to demonstrate that gold nanoparticles functionalized with a mixed-monolayer of hydrophobic and hydrophilic alkanethiol ligands can act as synthetic analogues of these fusion proteins and mediate lipid membrane fusion by catalyzing the formation of a toroidal stalk between adjacent membranes and enabling the formation of a fusion pore upon influx of  $\text{Ca}^{2+}$  into the exterior solvent. The fusion pathway enabled by these synthetic nanostructures is analogous to the regulated fast fusion pathway observed during synaptic vesicle fusion; it therefore provides novel physical insights into this important biological process while also being relevant in a number of single-cell therapeutic applications.

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