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Forming of Janus Particles by Surface Adsorption of Biomolecules

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Janus particles possess two or more distinct properties on their surfaces. This asymmetric surface structure leads to interesting properties and enables potential applications in biomedical and biological fields. In this presentation, we focused on the competitive adsorption process of Au/PS Janus particles. Based on experimental observations, we used a coarse-grain molecular dynamics (CGMD) model to seek mechanistic explanation of forming of Janus-type surface structures.

Coarse-grain molecular dynamics model assumes competitive adsorption of different molecules onto the gold surface and diffusive phase segregation. Once the DNA-thiol and lipid-thiol randomly adsorb to the surface of gold nanoparticle, the self-assembly reaction begins due to the affinity of thiol functional groups with gold, and their mobility as a small molecule. It is assumed that there will be a time window for the two to molecules to relocate on the surface of the nanoparticle and segregate into two regions before PAN-PS polymer is attached to the lipid-thiol molecule. The driven force for the segregation is to decrease the interface energy between the DNA and lipid groups.

Our simulations suggest that the two regions with different properties would not form two hemispheres. The interface between regions of different properties is more likely to be a curve similar to that on a tennis ball or baseball. This result may be explained by the Earth Mover's Distance in graph theory, i.e., the shortest overall distance travelled by all molecules from one configuration to another. Fig 1(a) is a feasible Janus particle configuration obtained by the coarse-grain MD simulations. Fig 1(b) shows transmission election microscopy (TEM) images of experimentally obtained Janus particles. Fig 1(c) shows possible TEM images of the Janus particle configuration in Fig. 1(a) from different perspectives. The results show that Janus particles that appear to be different in TEM images – some covered more than half by polymer, while others less than half – may be an artifact of being observed from different perspectives. Furthermore, although an ideal Janus particle configuration of two half spheres might be

thermodynamically preferred, a graph theory analysis shows that the tennis ball type configuration is kinetically favored.

Conclusions: A systematic numerical analysis has been conducted to study the mechanisms of the forming of Janus particles. From TEM images of experimentally fabricated particles and the results of CGMD simulations, we believe a curved interface between the two phases on a Janus particle similar to that on a tennis ball or baseball is feasible and can provide a consistent explanation of the observed TEM images of Janus particles. The research has the potential to provide an insight into the nanoscale structure of Janus particles that allows for further exploitation of its properties and leads to novel applications.

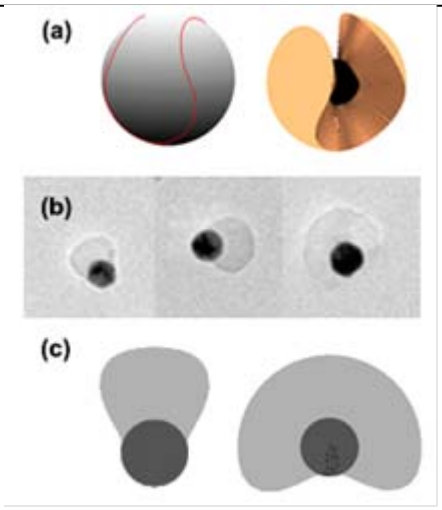

Figure 1. (a) Proposed configuration. The left figure depicts the boundary between the two regions, where the right has got the polymer attached (polymer is colored yellow, and the gold nanoparticle is the black core). (b) TEM image of the actual particles. (c) Simulated TEM image using the proposed configuration.