Tailoring Janus swimmers by mesoscopic simulations

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Active matter is one of the most exciting fields in statistical mechanics and materials engineering. Thanks to the groundbreaking work of synthetic chemists and material scientists, there is now a continually growing library of synthetic microswimmers and active colloids. These active particles are the synthetic analogs of swimming bacteria, but the synthetic variants have the advantage of tuning systematically both the inter-particle interactions and the hydrodynamic signature of the colloids.

Due to their non-equilibrium nature, most cases of active systems develop emergent behaviors such as collective motion, orientational order or *living clusters*. Some of us have already studied living cluster formation [1], where we have focused on the influence of the hydrodynamic interactions and the competition between the swimming velocity and the interaction strength among active particles with an attractive and isotropic potential, more recently, some of us have also studied the effect of a anisotropic potential in the formation of self-assembled states [2] using active amphiphilic dry colloids. Both studies help to understand in a systematic way, how active and hydrodynamic forces can be exploited in conjunction with anisotropic pair interactions to design macroscopic assemblies with desired structural properties.

Our current research focus on study systematically active amphiphilic swimmers, where in one hand, we have carried out Lattice Boltzmann simulations to model explicitly the swimmers hydrodynamics and on the other hand, we have carried out Brownian dynamics simulations to study systems where temperature plays a role but hydrodynamics interactions are absent.

To model swimmers we have used squirmer model, while the direct interaction between a pair of squirmers has been model in general by a pair-wise potential that depends on the the center-center distance and their attractive patch orientation

$$V(\vec{r}_{ij}, \hat{p}_i, \hat{p}_j) = V_{\text{rep}}(\vec{r}_{ij}) + V_{\text{att}}(\vec{r}_{ij})\phi(\theta_i, \theta_j), \qquad (1)$$

where $\hat{p}_i$ and $\hat{p}_j$ are the attractive patch directions of the particles i and j, respectively, while θ_i and θ_j are their relative orientations with respect of their patch direction. This potential is composed by two short range potentials: one very short-range repulsive part $V_{\text{rep}}(\vec{r}_{ij})$ and an attractive term $V_{\text{att}}(\vec{r}_{ij})$, the range of the attractive potentials is a parameter we have studied in this investigation.

A sketch of the two main cases of Janus swimmer pairs can be seen in Fig. 1: when a particle swim in the direction of the attractive patch, it calls *with the patch* swimmer (WP), while a particle swimming against the patch, it is called *against the patch* swimmer (AP). Another important parameter we have studied is the nature of the orientational part of the potential $\phi(\theta_i, \theta_j)$, which models the amphiphilic feature of the swimmers. We have used two models: one with

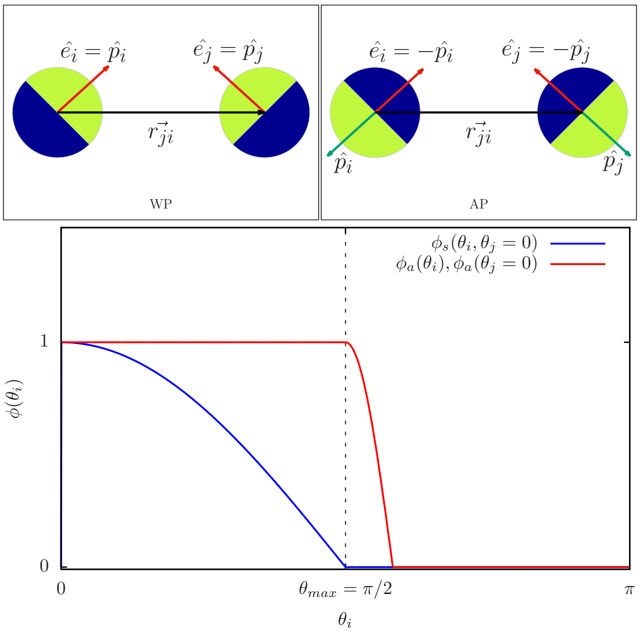

Fig. 1. Upper panels are sketches of the interaction between two Janus swimmers, attractive patch is in green, while non attractive patch is in blue. The direction of the swimming is represented by a red vector $\vec{e}$, the green vectors represent the direction of the attractive patch $\vec{p}$ and the black vector is the center-center distance between two swimmers $\vec{r}_{ij}$. Bottom panel is the graphic representation of the angular part of the Janus potential $\phi(\theta_i, \theta_j)$ in Eq. (1). Blue curve is used in Ref. [3], while red curve is used in Ref. [4].

non-zero torque within the interaction range (blue curve of the bottom panel in Fig. 1) and another one with non-zero torque just around the maximum relative angle between a pair of swimmers (red curve of the bottom panel in Fig. 1).

We have carried out systematic simulations of Janus swimmer suspensions changing the parameters described above. We have characterized the morphology, alignment and dynamics of the self-assembled states and living clusters observed, in order to elucidate the fundamental ingredients needed to design better macroscopic assemblies that could help to design new materials and micro-robots.

[1] F. Alarcón, C. Valeriani, and I. Pagonabarraga, Soft Matter, **13**, 814-826 (2017).

[2] S. A. Mallory, F. Alarcon, A. Cacciuto, and C. Valeriani, New J. Phys. **19**, 125014 (2017).

[3] L. Hong, A. Cacciuto, E. Luijten, and S. Granick, Langmuir **24**, 621-625 (2008).

[4] W. L. Miller and A. Cacciuto, Phys. Rev. E **80**, 021404 (2009).