Literature Reading & Review

Synthetic Chemotaxis and Collective Behavior in Active Matter

Published as part of the Accounts of Chemical Research special issue "Fundamental Aspects of Self-Powered Nano- and Micromotors".

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ACCOUNTS
of chemical research

Article

Cite This: *Acc. Chem. Res.* XXXX, XXX, XXX–XXX

pubs.acs.org/accounts

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1. Liebchen, B.; Cates, M. E.; Marenduzzo, D. Pattern formation in chemically interacting active rotors with self-propulsion. Soft Matter 2016, 12, 7259.
2. Liebchen, B.; Marenduzzo, D.; Cates, M. E. Phoretic interactions generically induce dynamic clusters and wave patterns in active colloids. Phys. Rev. Lett. 2017, 118, 268001.

Background
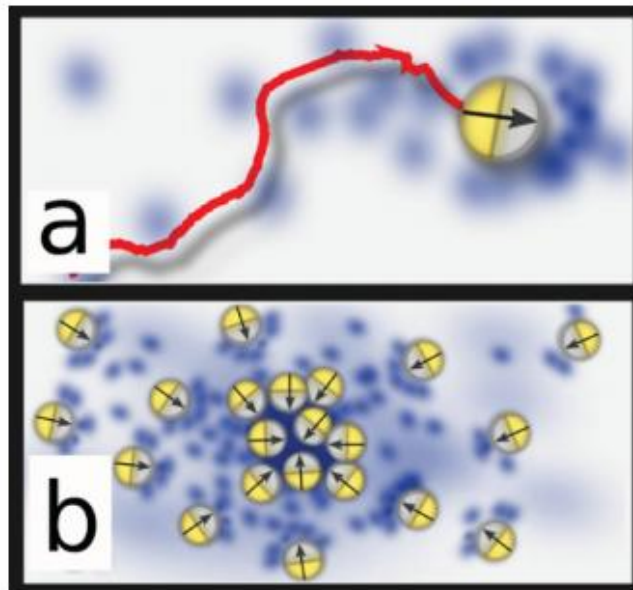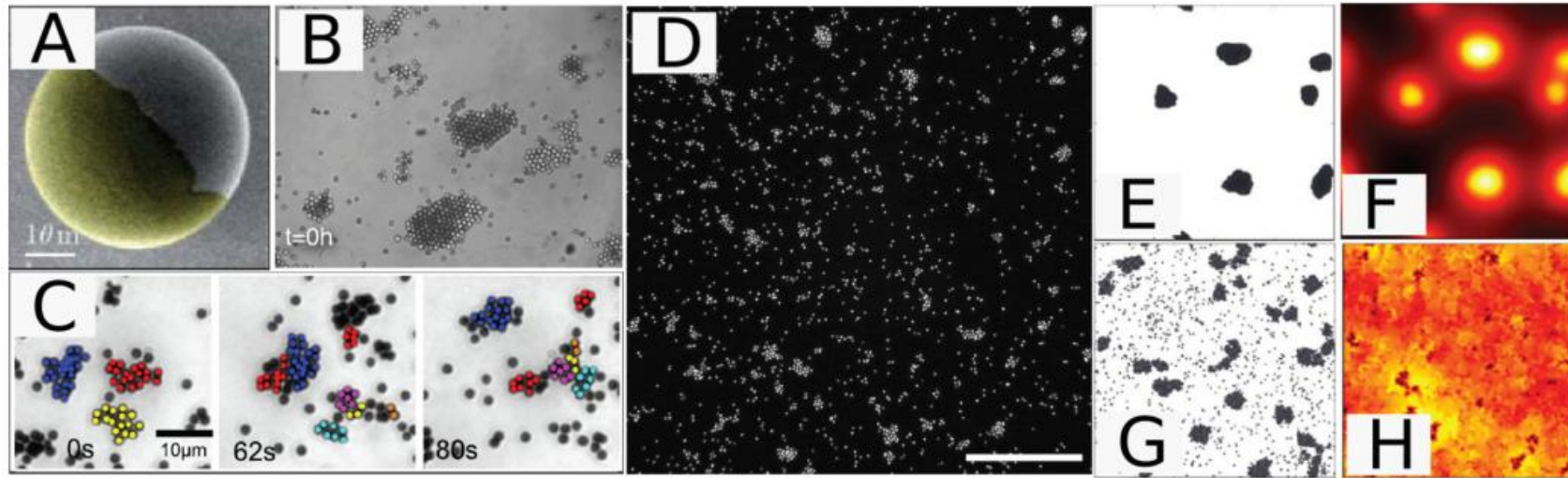
- Self-propelled
- Instability (swarming)
- Interaction fields
- Self-produced
- Taxis (chemotaxis, thermotaxis, phototaxis, viscotaxis(viscosity))
- Dictyostelium, autoinducers
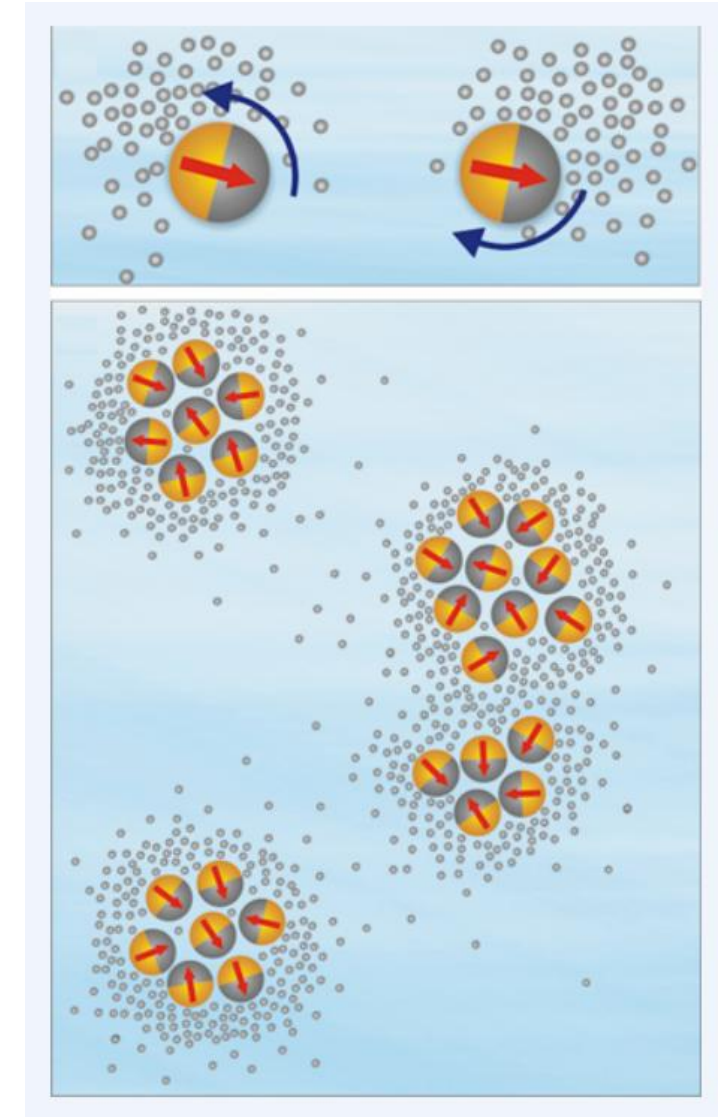
CHEMOTAXIS IN ISOTROPIC PARTICLES

One Particle

$$\dot{\mathbf{r}}_1(t) = \beta_D \nabla c(\mathbf{r}_1(t), t) + \sqrt{2D}\,\boldsymbol{\xi}(t)$$

the diffusion coefficient of the particle. If $\beta_D > 0$, the particle moves toward high chemical concentration and shows *chemoattraction* (or positive chemotaxis); if $\beta_D < 0$, the particle moves down the chemical gradient representing *chemorepulsion* (or negative chemotaxis).

As we have discussed above, many microorganisms self-produce the chemical to which they respond, say with a rate k_0. This is called (positive or negative) *autochemotaxis*. We

$$\dot{c}(\mathbf{r}, t) = D_c \nabla^2 c(\mathbf{r}, t) + k_0 \delta(\mathbf{r} - \mathbf{r}_1) - k_d c(\mathbf{r}, t)$$

taking place in the underlying solvent. For autochemoat-traction ($\beta_D > 0$), where the particle produces a chemical to which it is attracted, eqs 1 and 2 can lead to self-trapping in one and two dimensions (but not in three),[51] which can be permanent ($k_d = 0$[51]) or transient ($k_d > 0$[52,53]) and is opposed by noise.[54] Conversely, autochemorepulsion ($\beta_D < 0$) can lead to self-avoidance.[52,53] A system of two chemotactic particles, A

Collective Behavior: Keller–Segel Model

$$\mathbf{r}_1(t) \Rightarrow \mathbf{r}_i(t)$$

$$k_0 \delta(\mathbf{r} - \mathbf{r}_1(t)) \Rightarrow \sum_{i=1}^{N} k_0 \delta(\mathbf{r} - \mathbf{r}_i(t))$$

$$\rho(\mathbf{r}, t) \Rightarrow \sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i(t))$$

$$\dot{\rho} = -\nabla \cdot (\beta_D \rho \nabla c) + D \nabla^2 \rho$$

$$\dot{c} = D_c \nabla^2 c + k_0 \rho - k_d c$$

These equations represent the classical Keller–Segel model (see ref 21 for variants of this model). One obvious solution is $(\rho, c) = (\rho_0, k_0 \rho_0 / k_d)$ representing a uniform disordered phase. Performing a linear stability analysis of this phase predicts a criterion for the onset of structure formation, which reads:

$$\dot{\rho}' = -\beta_D \rho_0 \nabla^2 c' + D \nabla^2 \rho'$$

$$\dot{c}' = D_c \nabla^2 c' + k_0 \rho' - k_d c'$$

$$k_0 \rho_0 \beta_D > D k_d \tag{5}$$

CHEMOTAXIS IN ACTIVE PARTICLES
Active Particles in Imposed Gradients

$$\dot{\mathbf{r}}(t) = \nu_0 \mathbf{p} + \beta_{\mathrm{D}} \nabla c \left(\mathbf{r}(t), t\right) + \sqrt{2D}\,\boldsymbol{\xi}(t)$$

$$\dot{\theta}(t) = \beta \mathbf{p} \times \nabla c \left(\mathbf{r}(t), t\right) + \sqrt{2D_{\mathrm{r}}}\,\eta(t)$$

$$\mathbf{p} = (\cos\theta,\ \sin\theta)$$

$$\mathbf{a} \times \mathbf{b} = a_1 b_2 - a_2 b_1$$

$\beta > 0$ attractive	$\nu = -1$ cap ahead	$\beta > 0\ \ \nu = -1$ KS+Janus	$\beta > 0\ \ \nu = 1$ KS
$\beta < 0$ repulsive	$\nu = 1$ cap behind	$\beta < 0\ \ \nu = 1$ Delay+Janus	$\beta < 0\ \nu = -1$ Delay
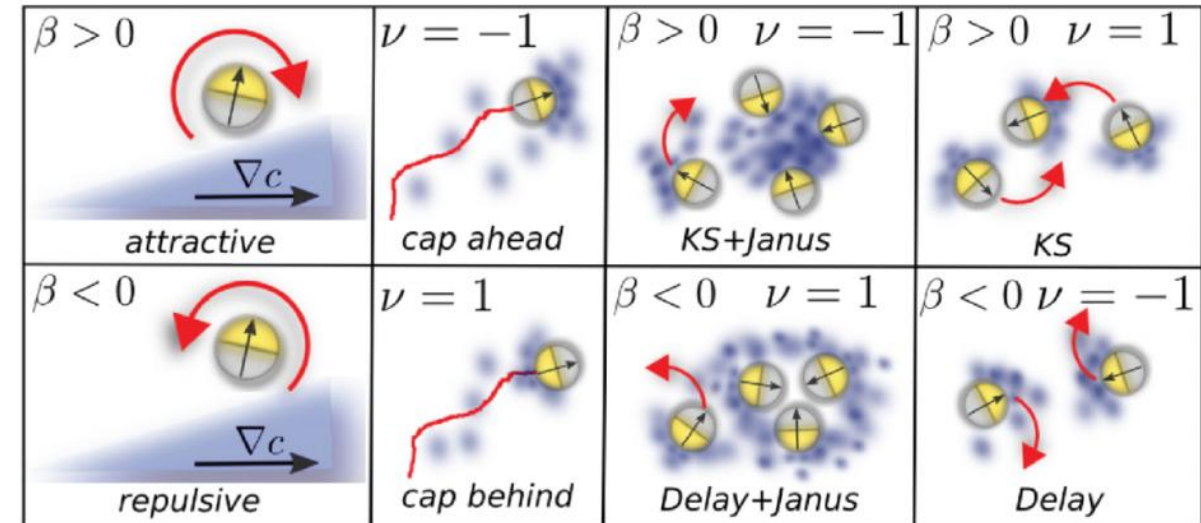
Collective Behavior: The Phoretic Brownian Particle Model

$$\dot{\mathbf{r}}_i = \nu_0 \mathbf{p}_i$$

$$\dot{\theta}_i = \beta \mathbf{p}_i \times \nabla c\left(\mathbf{r}_i\right) + \sqrt{2D_{\mathrm{r}}}\,\xi_i(t);\ \ i = 1,\ldots,N$$

$$\dot{c}(\mathbf{r}, t) = D_{\mathrm{c}} \nabla^2 c(\mathbf{r}, t) - k_{\mathrm{d}} c(\mathbf{r}, t)$$

$$+ \sum_{i=1}^{N} \oint d\mathbf{x}_i \delta\left(\mathbf{r} - \mathbf{r}_i(t) - R_0 \mathbf{x}_i\right) \sigma(\mathbf{x}_i)$$

(i) Since "active diffusion" dominates over passive diffusion, that is, $\sim v_0{}^2/D_{\mathrm{r}} \gg D$, we set $D \to 0$ in eq 6.

(ii) For simplicity, we also neglect the chemotactic drift ($\beta_{\mathrm{D}} \to 0$), allowing us to capture most aspects of chemically interacting microswimmers in a simplified way. (Physically, drift effects are also important for typical Janus colloids[35] but can to some extend be absorbed in the alignment effects we discuss here.)

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The Model

Field Theory of the Phoretic Brownian Particle Model

$$\rho(\mathbf{r},t) = \sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i(t))$$

$$\dot{\rho} = -\mathrm{Pe}\nabla \cdot \mathbf{w}$$

$$\mathbf{w} = \sum_{i=1}^{N} \mathbf{p}_i \delta(\mathbf{r} - \mathbf{r}_i(t))$$

$$\dot{\mathbf{w}} = -\mathbf{w} + \frac{B\rho}{2}\nabla c - \frac{\mathrm{Pe}}{2}\nabla\rho + \frac{\mathrm{Pe}^2}{16}\nabla^2\mathbf{w} - \frac{B^2|\nabla c|^2}{8}\mathbf{w}$$

$$+ \frac{\mathrm{Pe}B}{16}\left(3(\nabla\mathbf{w})^{\mathrm{T}} \cdot \nabla c - (\nabla c \cdot \nabla)\mathbf{w} - 3(\nabla \cdot \mathbf{w})\nabla c\right)$$

$$t_u = 1/D_r$$

$$x_u = R_0$$

$$\dot{c} = \mathcal{D}\nabla^2 c + K_0\rho + \nu\frac{K_0}{2}\nabla \cdot \mathbf{w} - K_{\mathrm{d}}c$$

Peclet number $\mathrm{Pe} = v_0/(R_0 D_r)$

$$B = \beta/(D_r R_0^4)$$

$$K_0 = k_0/D_r$$

$$\mathbf{w} \to 0, \dot{\mathbf{w}} = 0 \Rightarrow \mathbf{w} = \frac{B\rho}{2}\nabla c - \frac{\mathrm{Pe}}{2}\nabla\rho$$

$$K_d = k_d/D_r$$

$$\mathcal{D} = D_c/(R_0^2 D_r)$$

$$\frac{K_0\rho_0 B}{K_{\mathrm{d}}\mathrm{Pe}} > 1$$

$$\boldsymbol{\rho} = x_u^2 \mathbf{N}/L^{\mathbf{2}}$$

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Parameter Collapse and Universality

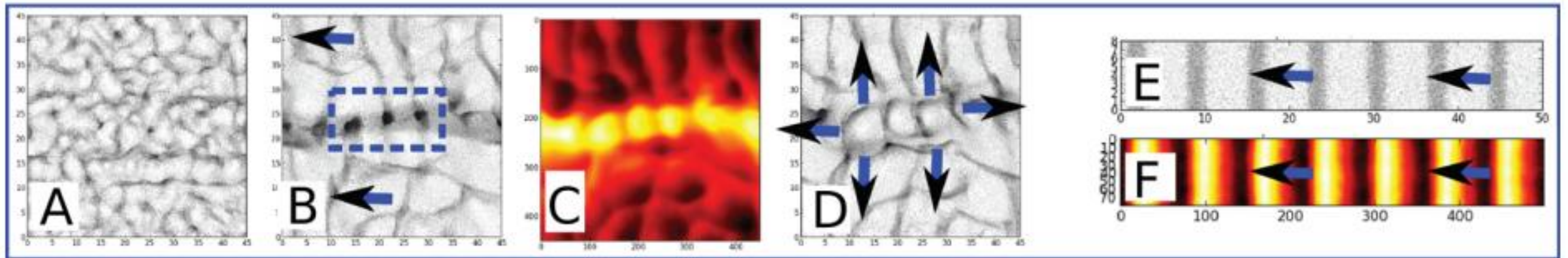$$\frac{K_0 \rho_0 B}{K_d \mathrm{Pe}} > 1$$

$$B \approx \frac{4\pi s\, \mathrm{Pe}\, \mathcal{D}}{K_0}$$

$$6\mathcal{D}f > K_d \quad (f = \pi R_0^2 \rho_0)$$

Chemorepulsive Route to Pattern Formation

$$K_d \ll 1 \Rightarrow 3\mathrm{Pe}f\left(\frac{v}{2} + \mathrm{Pe}\right) \gtrsim 1$$

- **Janus instability:** The first part of the criterion reads $3\mathrm{Pe}f\nu > 2$. Since $\nu = 0$ for isotropic chemical production on the surface of the particles, this criterion can only be fulfilled for anisotropic chemical production; hence it is called, the *Janus instability*. The Janus instability leads to clusters of finite size. The underlying physical mechanism is illustrated in Figure 5A.
- **Delay-induced instability:** The second criterion, $3\mathrm{Pe}^2 f > 1$, in eq 17 represents an oscillatory instability and creates wave patterns. The underlying delay-induced instability mechanism is detailed in Figure 5B.

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The Model

BEYOND THE ACTIVE BROWNIAN PARTICLE
MODEL: CHIRALITY

$$\dot{\rho} = -v_0 \nabla \cdot (\rho \mathbf{p}) + D_\rho \nabla^2 \rho + K \nabla^2 \rho^3$$

$$\dot{\phi} = \omega + \beta \mathbf{p} \times \nabla c$$

$$\dot{c} = k_0 \rho - k_d c + D_c \nabla^2 c + \epsilon (c - c_0)^3$$

$$\dot{\mathbf{r}}_i = v_0 \mathbf{p}_i$$

$$\dot{\theta}_i = \Omega_i + \beta_R \mathbf{p}_i \times \nabla c$$

$$+ G \sum_{j=1}^{N} \sin(\theta_i - \theta_j) \delta(\mathbf{r}_i - \mathbf{r}_j) + \sqrt{2D_r} \, \xi_i(t)$$

$$\dot{c} = k_0 \sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i) - k_d c + D_c \nabla^2 c + \epsilon (c - c_0)^3$$