

Chemical Physics of Active Matter

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Active matter composed of self-propelled particles has become an increasingly topical research arena in the field of nonequilibrium phenomena. Fascinating new physics, such as spontaneous collective motion and motility induced phase separation, have been reported and studied extensively. In the past 20 years, significant progress has been enabled by the joint study of model experimental systems (e.g., synthetic microswimmers, motile colloidal particles, micro-organisms, or vibrated granulates), simulations of simplified models, and theoretical analysis ranging from kinetic to field theories.

Self-propelled particles that are perpetually moving by converting energy (“fuel”) into mechanical motion are intrinsically nonequilibrium systems. These particles are the building blocks of a new material class called “active matter,” which exhibits a plethora of fascinating properties absent from ordinary equilibrium matter as well as from matter driven out of equilibrium by external gradients. The underlying motivations of the active matter research in the last decades are twofold: first, there is a broad range of applications, such as precision surgery, drug delivery, and cargo transport on the micrometer scale, where active particles have to navigate through a disordered environment, often filled with a complex medium. Second, and maybe more importantly, a fundamental understanding of the novel phenomena requires systematic experiments, new modeling, and theoretical descriptions beyond equilibrium or close to equilibrium physics. One of the first standard models in this respect is the Vicsek model of swarming proposed in 1995 by Vicsek and co-workers,¹ which is by now a cornerstone in describing collective active matter systems. With the upsurge of synthetic colloidal Janus-like particles, which create their own gradient in which they are moving, artificial microswimmers were considered as model systems for active matter. These micrometer-sized particles typically self-propel in a liquid at very low Reynolds number. A wealth of novel effects was discovered, in particular new nonequilibrium states like clustering, swarming, chaotic flows, and motility-induced phase separation. Active matter research is highly

interdisciplinary, nested between statistical physics, chemistry, fluid mechanics, and biology. Several reviews on this rapidly growing field are available.^{2–6}

While the motion of single particles in Newtonian solvents is by now well understood, future perspectives include active particle motion in more complex environments, such as external fields and disordered media. Collective motion in dense active systems, where crystallization, jamming, and glass formation may develop, is also a promising research pathway. On the theoretical side, understanding the statistical mechanics and the thermodynamic foundations of active matter is of prime interest. This special topic summarizes recent advances in our understanding of active matter highlighting the interplay between experiment, simulation, and theory. This special topic summarizes recent progress in our understanding of active matter. There are in total 44 papers^{7–50} and we briefly comment in this editorial on the scientific questions posed and on the advances of this field in general.

The major part of papers in this special topic concerns theory and simulations but there are also experimental papers. This reflects well the general trend in the field of active matter where there are many more theoretical and simulation studies than actual experiments. In detail, on the one hand, there are about 27 papers where theoretical aspects of active matter are discussed^{7–44} and 19 papers which involve simulations.^{7,12,16,18,21,24,28,32–43} On the other hand, there are 7 experimental studies concerning artificial colloidal Janus particles,^{18,35,43,44,50} microalga,⁴⁷ and enzymes.⁴⁸ Finally, one paper is concerned with statistical analysis of experimental data.⁴⁹

Regarding the modeling of active particles there are different levels: beyond the Vicsek model,¹ the simplest model is the active *Ornstein-Uhlenbeck particle* (AOUP), which has just translational degrees of freedom with some kind of translational memory establishing a persistence in its motion with a characteristic persistence length. The AOUP has the advantage that some of its properties are

analytically soluble; the disadvantage is that it is a rather crude model for details of an active particle. Two of the papers^{7,28} in this special topic are using the AOUP model. On the next level, there is the standard *Active Brownian Particle* (ABP) model coupling orientational and translational degrees of freedom. An ABP self-propels along its orientation and possesses a persistence in its motion set by the orientational noise. Since the particle is polar, the ABP model is more detailed than the AOUP model. The ABP model has now become the standard model to study active matter since it can be simulated easily and it is realized for synthetic colloidal Janus-particles if hydrodynamic interactions are ignored. In fact, many papers in this special topic use ABPs to describe and predict single and collective phenomena of active particles.^{10,15,18,22,23,38} On a similar level, there are run-and-tumble models which involve an explicit run and tumble step. These models are more appropriate for bacteria and are considered in Refs. 16 and 41. When the hydrodynamics of the supporting medium is incorporated,^{8–10,20,30,42,44} the description becomes much more involved, and several papers specifically address this issue.^{10,42,44}

While most of the studies done so far were conducted using colloidal Janus particles, other particle types are proposed and discussed in this special topic. They include active droplets,^{8,30} active colloidal molecules made up of active and passive constituents,³⁵ and chains of active colloids, also called active polymers.¹⁵ On the biological side one finds here studies dealing with algae,⁴⁷ cells,⁴⁹ and enzymes.^{20,48} Several mechanisms of self-propulsion are discussed; phoretic effects,^{8,9} light activation,¹⁹ and electrochemical effects were considered to control the self-propulsion of micro-motors.⁴⁵ Also, particles can not only propel translationally but also spin, such as rotorlike active particles,⁴⁶ thereby opening new promising research routes.

One important step forward beyond the study of a single active particle moving on a two-dimensional substrate is to add an *external field* and to study the particle's response to this field. This response can be counterintuitive and is, therefore, under intense exploration. This special topic contains several key examples. There are new aspects of active sedimentation under gravity,³⁴ and a brazil-nut-like effect was discovered in active binary mixtures, where the heavier particles float on top of the lighter ones.¹⁸ An imposed shear flow of the supporting solvent is another external field to which active particles respond to, as discussed in Ref. 17. Particle crossing over an external potential barrier, i.e., the famous Kramers problem for passive particles, constitutes another fundamental topic^{7,27} and has applications in the understanding of the penetration of active particles through elastic membranes¹² or the motion of a biological swimmer in a patterned environment.⁴⁷ Finally a theoretical study revealed how particle can be steered by an oblique light illumination.¹⁹

If it comes to *interactions between active particles*, the first element of classification to think of is whether they are aligning or non-aligning. Typical ABPs are considered without aligning interactions. Including alignment can drastically change effects as exemplified for motility-induced phase separation.⁴⁰ A crucial point, which is still under debate and is discussed in this special topic in Refs. 8–10, 31, and 32, is the coupling between hydrodynamics and advection diffusion of chemicals, when the active particle is guided by chemotaxis, i.e., by sensing a chemical which is generated by neighboring particles or by itself.^{9,10,20}

Depending on the interactions, rich *collective phenomena* are found, and many examples are discussed in this special topic. While the transition to collective motion in dilute phases was the central topic in the early ages of the field, recent studies focus on the denser phases of active matter. Theories for the glass and jamming transition in active systems have been proposed by extending mode coupling and other approaches toward active particles. A review and perspective paper on this topic is proposed⁴³ and the details of a mode coupling theory are discussed.²² The liquid state theory and a study of pair correlations are conducted in Refs. 13 and 42, and several aspects of the motility-induced phase separation are discussed.^{18,25,40} Crystallization also turns out to be subtle in two spatial dimensions due to an intervening hexatic phase,³⁷ and activity also opens the way toward novel phenomena like sculpting of colloidal crystals.²³

Another promising avenue of recent research is provided by *mixtures of active particles* at finite density, for example, binary mixtures of active and passive particles. The emerging behavior is in general much more complex than that for one-component systems as exemplified by several studies in this special topic.^{10,18,24,33}

Also, the polar nature of active matter provides a platform to display novel *topological effects*, and two examples are put forward in this special topic: the formation of active skyrmions (known as such from spin vortices of passive condensed matter systems)¹⁴ and active topological defects in cellular structures.³⁹

Finally, *fundamental questions of statistical physics* are discussed in this special topic as well. The specificity of active matter is that the dynamics of the individual component violate detailed balance. The mapping onto effective equilibrium systems is discussed,²⁸ but there are several caveats in doing so, as exemplified in the role and definition of the chemical potential in nonequilibrium.¹⁶ The polar phase of aligning active particles develops very specific fluctuations, the so-called giant number fluctuations,²⁶ raising questions about large deviations in such systems. A generalization of the fluctuation-dissipation theorem toward finite activity²⁹ is considered and studied in this special topic as well.

Altogether, the present special topic clearly demonstrates that the field of active matter has left its infancy, when the primary concern was the study of the transition to collective motion in systems of polar aligning particles. The diversity of systems studied experimentally, from the enzymatic molecules to the macroscopic living species, including hand-made self-propelled colloids, together with the emergence of more general questions, such as the nature of dense phases, and the relevance of a thermodynamics description, has conducted the research in active matter toward a highly interdisciplinary research topic, with many opportunities from both the fundamental and the application viewpoints. A lot remains to be done, and it is our best wish that the present collection will motivate young researchers to join in this research topic, characterized by its high ratio of unexpected over expected results.

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