Active nano/microsystems in the Spanish context

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Book of Abstracts

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Brownian dynamics and spontaneous rotation of a Janus particle in a polymer solution

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The development of engineered active colloids that harness the chemical energy of the environment to move has enabled one to mimic and dissect mechanisms in biological systems while opening doors to multiple applications: bioremediation, micromixing, micromachinery, drug delivery, and more. However, the application of active colloids for biomedical applications must consider the complex nature of most biological fluids, which contain large macromolecules and display viscoelastic and non-Newtonian rheology.
Recent experiments showed that active colloids propelling through a polymer solution experience a drastically enhanced rotational diffusion and can rotate spontaneously due to an instability the origin of which is not understood. Earlier work suggests that the instability arises from the advection of polymers around the colloid and requires a fore-aft asymmetric interaction between the particle and the polymers.
Here, we go beyond the study of the instability and we employ a fluctuating hydrodynamics approach developed in our group to study the Brownian dynamics and the spontaneous rotation of a spherical Janus active particle moving through a polymer solution. We model the evolution of the polymer concentration using a stochastic advection-diffusion equation that includes the thermal fluctuations of the polymer concentration. The results show that driving a Janus particle out of equilibrium in a polymer solution has a profound impact on its Brownian dynamics. In agreement with the experiments, we find that the rotational diffusion coefficient is drastically enhanced before the onset of the spontaneous rotation. Our work demonstrates the importance of considering the colloidal nature of polymer solutions and highlights the challenges of controlling active matter in a complex fluidic environment.

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Tailored Polymeric Nanocontainers: Adjusting Permeability and Function

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In next-generation therapeutics and synthetic biology, nanoreservoirs with enzyme-like activity are gaining attention for their potential to replace biological functions, introduce new cellular capabilities, or control therapeutic effects. These artificial cell nano-structures hold promise for enhancing targeted therapies, biosensor platforms, and modulating immune responses. For instance, manipulating reactive oxygen species (ROS) through the Fenton reaction could lead to advanced materials, though controlling ROS generation remains a challenge for safety and efficacy.

In this framework, we have previously described ferrocene-containing polymersomes (FcPsomes) with ferrocene units in their membrane, demonstrating their capacity for radical generation and

enzyme-mediated cargo release,[1],[2] promising features to promote combined effects in a single nanoplatform, scale them up to more complex systems and make a significant contribution to the nanocatalic medicine. Later, we have made significant progress by improving the fabrication, resulting in more uniform nanoscale self-assembled structures capable of loading bio(macro)molecules and adapting membrane properties to the biological environment. Using a tailored mixture of pH-responsive block copolymers (BCPs), we have developed photo-crosslinked and pH responsive polymersomes with ferrocene units, which provide distinct therapeutic windows dependent on pH and salt concentrations. Deep structural-function characterization study has been conducted, biomimetic approaches and preliminary cancer therapy tests. Lastly, integrating these nanoreservoirs with active matter systems could lead to dynamic materials, including functionalized micromotors for precise drug delivery and overcoming biological barriers.[3]

References
[1] Moreno, S; Hübner, H; Effenberg, C; Boye, S; Ramuglia, A; Schmitt, D; Voit, B, Weidinger, I; Gallei, M, *Appelhans, D* Biomacromolecules 2022, 23, 11, 4655-4667.
[2] Wang, D; Moreno, S*; Boye, S; Voit, B; Appelhans D* Macromol. Rapid Commun. 2023, 44, 2200885.
[3] Rajabasadi, F; Moreno, S; Fichna, K; Aziz, A; Appelhans, D; Schmidt, O. G.; Medina-Sánchez, M Adv. Mater. 2022, 34, 50, 2270346.

Coffee Break / Poster Session / **4**

Hydrodynamic viscous levitation of magnetically driven S-shape propellers

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Hydrodynamic interactions (HIs), namely solvent-mediated long-range interactions between dispersed, microscopic particles, play a crucial role in the emergent dynamics of many active systems, from swimming bacteria to swarms of propelling microrobots. For example, HIs forces the bacteria E. Coli tend to swim close to a surface, where it performs a circular trajectory nearby. The attraction results from the pusher type force dipole of the bacteria, which creates a flow field able to force the bacteria towards the wall. Similarly, for a puller type swimmer, the generated flow field induces a repulsion from the wall. However, for pullers, the alignment parallel to the wall is not a stable configuration. Inspired by this effect, we design a microscale magnetic rotor able to produce a puller-like force dipole, but with a stable alignment parallel to the wall.

These S-shape lithographic particles are doped with nanoscale magnetic colloids and can be manipulated via external, time-dependent magnetic fields. Under a rotating, circularly polarized magnetic field, these propellers are subjected to a magnetic torque, and rotate exerting a force on the surrounding fluid. Because of the anisotropy of the drag coefficient on the elongated shape, similar to a pusher type bacterium, a pair of forces arise pointing towards the center of mass of the particle. Since the S-shape rotates above a wall, it experiences an upward lift force. We optimize the shape of the S particle to maximize the lift force. Since the lift force decreases with the distance from the wall, we calculate the equilibrium rotation height for different rotation frequencies. We find that an S-shaped particle with the cross-section radius of 3 microns and the length of 120 microns lifts to a height of around 100 microns when rotated at a frequency of 6 Hz in water-glycerol mixture with the viscosity 9.7 mPa s.

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Modulation of Amyloid-β Aggregation with Metal Nanoparticles

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Conformational pathologies, including neurodegenerative ones, are characterized by misfolded proteins called amyloids, which lose their physiological role and acquire toxicity. The accumulation and spread of amyloids is related to an impaired proteostasis network. Chaperones, as key actors of proteostasis, have thus become promising drug targets and models.
We are exploring how metal nanoparticles might be used to either emulate or assist natural chaperones' action against amyloid accumulation in Alzheimer's disease.

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MOTION AND CONTROL OF VIRTUAL PARTICLES IN CONFINED CHIRAL LIQUID CRYSTALS

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Cholesteric phases are liquid crystals in which a helical twist can be induced by the presence of a chiral agent. This twist, with a periodicity or pitch (p), can be frustrated under geometrical confinement comparable to p. Under those conditions, skyrmions can be formed if the material undergoes an instability. Skyrmions are topologically protected solitonic-like structures [1-3], formed by the spatial discordance in the orientation of the molecules of the liquid crystal, forming a torus in which the principal axis of the molecules turns 180o. Skyrmions behave as quasi-particles and can be driven by the action of a modulated AC electric field [1-3]. However, the directionality of their motion has, so far, only been in-situ controlled using complex optical systems [3]. In our work, we study the propulsion of skyrmions under modulated AC electric fields of different amplitude, carrier, and modulation frequencies. We also demonstrate the capability of an external fixed magnetic field to steer driven skyrmions, which can be inserted and controlled within microfluidic channels. Experimental suggest an acceleration when skyrmions are introduced in micro-channels due to distortions in the LC molecular alignment generated by the presence of homeotropic walls. We also show that skyrmions can act as micro-cargo transporters.

[1] Shon, et. al., Nat. Commun, 10:14744 (2019), 1-11.
[2] Ackerman, et. al., Nat. Commun, 6:673 (2017), 1-13.
[3] Shon, et. al., Opt. Express, 28:5 (2020), 6306-6319.

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Innovative Lanthanide Polyoxometalates: Exploring Structural Diversity for Advanced Functional Materials

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Lanthanide polyoxometalates (Ln-POMs) have garnered interest due to their diverse structural motifs and potential applications in various fields. In this work, we report the synthesis and characterization of Anderson-type Ln-POMs, with the general formula $[Ln(H_2O)x]_2[TeMo_6O_{24}] \cdot yH_2O$, where Ln represents lanthanide cations (Tb^{3+}, La^{3+}, Dy^{3+}, Ce^{3+}, Sm^{3+}, Er^{3+}, and Gd^{3+}), x corresponds to the number of coordinated water molecules, and y denotes the number of lattice water molecules. These compounds crystallize in two distinct structural types: monomeric and ribbon-like frameworks. The monomeric structures are observed for Ln = Tb^{3+}, Dy^{3+}, and Er^{3+}, with x = 6-7 and y = 10-18. In contrast, the ribbon-like structures are found for Ln = La^{3+}, Ce^{3+}, Sm^{3+}, and Gd^{3+}, where x = 5-7 and y = 2-16.A notable feature of this study is the successful synthesis of the Gd^{3+}-based compound, $[(Gd(H_2O)_7]_2[TeMo_6O_{24}] \cdot 4H_2O$, via both slow evaporation and microwave-assisted methods, demonstrating the ability to retain the ribbon structure under varying synthetic conditions. Characterization was performed using single-crystal X-ray diffraction (S-XRD), powder X-ray diffraction (PXRD), and infrared spectroscopy, confirming the structural identity of the compounds. Future investigations will focus on exploring the magnetic properties and supercapacitor behavior of these Ln-POMs, which could provide insights into their potential applications in energy storage technologies and multifunctional materials.

Keywords: Lanthanide Anderson polyoxometalates (Ln- AndersonPOMs), Monomeric structures, Ribbon structures, Microwave-assisted synthesis, Supercapacitors, Energy storage

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Growing and Shaping Metal–Organic Framework Single Crystals at the Millimeter Scale

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Morphological control of crystals is utterly important in reticular chemistry, especially as a fundamental strategy toward preparing functional materials of superior properties. Despite the notable advancements in the realm of metal-organic frameworks (MOFs), where endeavors primarily focus on shape manipulation at the nano- and microscale during bulk synthesis and subsequent processing at the mesoscale (e.g., incorporation into polycrystalline films, patterns, and composites), a notable challenge persists in attaining a meticulous control over both the shape and size of macroscopic single crystals.
Here we successfully demonstrated the spatial and morphological control of crystal growth at the millimeter scale from a non-equilibrium state through the utilization of a microfluidic device. Specifically, we employed PDMS channels to confine CuGHG, a peptide-based MOF, where crystal formation occurred as a consequence of a diffusion-controlled supply of precursors within an advection-free microenvironment. Depending on the concentration of the feeding solution, continuous growth or shrinkage of the crystals was observed and recorded by time-lapse microscope. Our method not only introduces a novel approach for precisely shaping large-scale single crystals from metastable solutions but also draws attention to its intriguing resemblance to two fundamental morphogenesis strategies observed in biomineralization. The presented results, therefore, establish a fundamental basis for future studies in materials science, shedding light on how the size and shape of artificial crystals can intricately influence their properties and functions.Moreover, our findings provide a strategic avenue for tailoring the size and shape of peptide-based MOF single crystals to specific applications. This approach not only expands the horizons of crystal engineering but also opens up possibilities for the design and customization of materials with desired properties for various technological applications.

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Fuel Driven Dynamic Phospholipid Vesicles with Programmable Lifetime for Controlled Cargo Release

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Metabolic processes are crucial for sustaining life, involving the cyclic synthesis (anabolism) and degradation (catabolism) of chemical and supramolecular structures through the expense of chemical energy [1]. These highly dynamic structures which form under out-of-equilibrium (OOE) conditions define the hallmark features of life such as adaptivity and spatiotemporal control [2]. At the cellular level, metabolic activities govern functions by modulating phospholipid synthesis and breakdown. However, replicating synthetic vesicles that mimic cellular phospholipid membranes has proven difficult. In this work, we present a bioinspired approach for the in situ synthesis of biomimetic phospholipids and their self-assembly, driven by chemical fuel under physiological conditions, resulting in vesicles with a controllable lifetime. The phospholipids are formed via an amino-ester bond through imine formation (anabolic reaction), leading to spontaneous vesicle formation. In the presence of lipase, the ester bond is hydrolysed (catabolic reaction), triggering vesicle disassembly. Spectroscopic and microscopic analysis confirmed the continuous cycle of vesicle formation and breakdown. By varying lipase concentrations, we fine-tuned the vesicles'lifetimes, ranging from minutes to hours. Additionally, by supplying excess fuel, we sustained these dynamic vesicles in its assembly state. Detailed studies showed that the assembly can be temporally controlled by the amount of fuel supplied as well as the kinetics of the enzymatic reaction. We also demonstrated the potential application of these vesicles for drug release by encapsulating hydrophobic and hydrophilic model drugs and showed that the release kinetics of the encapsulated cargo molecules can be dynamically regulated for potential applications in adaptive nanomedicine.

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Emergence of a vortex lattice in anisotropic active flow under confinement

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We assemble a biomimetic active material from microscopic components like cells' filaments and protein motors that consume energy and generate continuous motion. Such active systems are capable of self-organization at different length and time scales, often exhibiting turbulent flows and the emergence of long-range orientational order, which is a characteristic of active nematics (AN). Previously, it was demonstrated that, by bringing into contact a two-dimensional AN with an anisotropic oil that features smectic liquid-crystalline order, it is possible to transform the originally turbulent flow of the active fluid into well-aligned flows ordered by a magnetic field [1]. Alternatively, the flow of active nematic could be controlled by confining walls [2] or arrangements of obstacles [3].
n present work we combine both approaches: well-aligned flows of AN ordered by a magnetic field were confined between walls of PDMS channels. The resulting quasi-laminar flows of AN are perturbed by closely located channel walls and reorganized in arrays of vortexes forming an hexagonal lattice. The emergence of vortex lattices is correlated with positional ordering of topological defects and the appearance of density patterns. The observed self-organization of the active flows is activity

dependent and reflects the inherent properties of the aligned AN. The described system is an example of pattern formation from instabilities of AN flows and suggests potential applications in the design and control of active materials.

[1] P. Guillamat, et al., Proc. Natl. Acad. Sci. U. S. A., 113, 20 (2016).
[2] J.Hardoüin et al., Soft Matter, 16, (2020).
[3] B. Zhang, et al., Phys. Rev. Research, 2, 4 (2020).

Coffee Break / Poster Session / 11

Bacteriabots as motile "stealth"biological carriers: characterization and perspectives

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During the last decade, many attempts have been made to develop new technologies capable of interacting with systems at very low dimensional scales, from nano to micrometers, and perform very specific tasks. Interest in this type of research arises from the possibility of conducting operations in a localized and controlled manner. One of the most promising among these technologies turns out to be the concept of Microswimmer, which belongs to the broadest class of active colloids. An active colloid is a suspension of particles capable of converting free energy from their environment into movement. Biological (Bacteria) and artificial (synthetic self-propelled particles) microswimmers are well-known examples of active colloidal systems. Microswimmers use the surrounding energy to carry out intrinsically non-equilibrium activities such as growth, replication and self-propelled motility [1]. Therefore, the way to arrive and operate in systems on the micro/nanoscale is to use materials characterized by a dimensional scale comparable to that of the systems with which they will interact. Considering this, microswimmers can be defined as very small objects, functionalized and optimized to perform specific actions through their movement, such as drug delivery, analyte detection or even antibacterial activity.
We present here a special case of biohybrid Microswimmers: the Bacteriabots; which result from the attachment of an inorganic functional particle (as cargo) to a motile bacteria (carrier) [2]. Accordingly, this communication includes the appropriate characterization of these materials using optical microscopy, electron microscopy and analysis of surface charge by Zeta Potential. Subsequently, characterization of the mobility of this class of active colloids is developed, specifically for the Bacteria and the Bacteria-Cargo. It is aimed to explain the different behavior observed in different study conditions, with future perspectives for applications in fields such as nanomedicine, electrochemical detection or antimicrobial agents.

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Magnetic (nano)actuators for enhanced mass transfer in voltammetric and spectroelectrochemical assays.

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Emerging Contaminants (ECs) are considered anthropogenic impact indicators, whose detection and quantification contribute to understanding their occurrence, distribution, and potential toxicity, allowing for effective mitigation strategies and environmental management. Electrochemical sensors based on screen-printed electrodes (SPE) have gained significant attention due to their advantages such as fast response, simplicity, sensitivity, cost-effectiveness and tuneability. In this sense, progress in nanomaterials preparation and modification strategies of SPEs leads to improved sensitivity and specificity, making these systems suitable for voltammetric detecting a wide range of ECs.
Other electrochemical methods to screen analytes and processes are Spectroelectrochemical (SEC) measurements in the UV-vis region. These are based on the changes that occur in the absorption spectrum of a liquid sample when an electrochemical process consumes or generates an absorbing species at the working electrode. In normal reflection mode, these measurements are less sensitive than those obtained in parallel configuration. This is because the monitored sample volume contains a much smaller diffusion layer created by the electrochemical processes, i.e. the region where the relevant optical changes take place. On the other hand, the standard configuration is more robust and reproducible and, currently, it is the only one commercially available.
In some cases, parameters such as repeatability, reproducibility and sensitivity seemed to be improved by the incorporation of magnetic cobalt ferrite nanoparticles into the measuring solution, acting as diffusion enhancers at the nanometric range.
This work describes a strategy to improve normal measurements in voltammetric and SEC analysis, The strategy is based on the addition of magnetic cobalt ferrite nanoparticles (MNPs) The induced movement of the MNPs (nano-enabled stirring) enhances the transport of matter to and from the electrode, producing a rapid renewal of the diffusion layer and, therefore, an increase in current signal.

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NEW INSIGHTS INTO SELF–PHORESIS

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Chemophoresis describes the displacement of a particle in an ambient fluid due to a gradient in chemical composition. Classic phoresis can be understood through linear-response theory: in the presence of a sufficiently small, externally imposed gradient $(\nabla n)_{\rm ext}$ in concentration, the phoretic velocity of the particle is $\mathbf{V} = \mathcal{L}_{\rm lin}(\nabla n)_{\rm ext}$, in terms of the phoretic coefficient $\mathcal{L}_{\rm lin}$ given by a Green-Kubo expression.

Self-phoretic particles induce a composition gradient $(\nabla n)_{\rm act}$ through catalytic activity and provide a physical realization of artificial swimmers. Experimental observations are then customarily addressed as another instance of classic phoresis, $\mathbf{V} = \mathcal{L}_{\rm lin}(\nabla n)_{\rm act}$.

However, an additional role of the particle's chemical activity has been recently identified as responsible for a specific activity-induced response $\mathcal{L}_{\rm act}$, so that one has to write $\mathbf{V} = (\mathcal{L}_{\rm lin} + \mathcal{L}_{\rm act})\,[(\nabla n)_{\rm ext} + (\nabla n)_{\rm act}]$ in the more general scenario. This means a change in paradigm as it disproves the claim that "self-phoresis is phoresis in a self-induced gradient".

- A. Domínguez, M.N. Popescu, C. Rohwer, S. Dietrich, *Phys. Rev. Lett.* **125**, 268002 (2020).
- A. Domínguez, M.N. Popescu, *Curr. Op. Coll. & Interface Sci.*, **61**, 101610 (2022).
- A. Domínguez, M.N. Popescu, *Mol. Phys.*, doi: 10.1080/00268976.2024.2396545 (2024).
- A. Domínguez, M.N. Popescu, *arXiv:2404.16435*
- A. Domínguez, M.N. Popescu, *arXiv:2407.08314*

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Dissipative self assembly of FtsZ over confined lipid bilayers

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FtsZ is a protein involved in bacterial cell division. This study examines the behavior of FtsZ under two-dimensional confinement and lateral spatial restrictions as an alternative to its three-dimensional confinement within a bacterium. Two protocols were developed to restrict the lateral movement of the protein in bilayers containing a lipid mixture of 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (POPC) with 5% Nitrilotriacetic acid (NTA).

The first protocol involves creating micrometer-sized corrals using bovine serum albumin (BSA) / Polyethylene Glycol (PEG)-impregnated seals on pre-cleaned glass, then introducing the bilayer into these corrals and adding the FtsZ protein. The second protocol uses bilayer islands generated from a solution of Giant Unilamellar Vesicles (GUVs) at very low concentration on an atomically flat mica surface.

Once FtsZ is confined in this two-dimensional setup, its behavior was studied using Atomic Force Microscopy (AFM). The results represent an advance in FtsZ confinement techniques, although significant challenges were encountered, particularly with the first method. The confinement allowed for observations of distinct behaviors in the folding and distribution of FtsZ, suggesting its ability to modify and generate NTA patches in the fluid bilayer. These findings open new possibilities for FtsZ confinement methods and the development of protocols to enhance understanding of its behavior in the bacterial membrane, contributing to insights into bacterial division mechanisms and potential antibiotic design.

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Squirmers at a fluid-fluid interface: anisotropic, compressible hydrodynamic interactions

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Squirmers provide a simple and effective model for active particles. We consider the particular case of shakers (non-self-propelling squirmers) confined to a fluid-fluid interface, so that an ultraconfined 2D colloid immersed in a 3D fluid is obtained. This dimensionally hybrid (2D/3D) configuration alters the hydrodynamic interactions significantly due to the symmetry breaking of the orientational isotropy of shakers and the effective 2D compressibility of the projected in-plane 3D flow. We study the collective dynamics of such system analytically and numerically, and we highlight some features following specifically from the modified hydrodynamic interactions.

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Integrating AFM in Nanomedicine: Biophysical Mapping for Diagnostics and Drug Delivery

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The atomic force microscope (AFM) is gaining progressive attention for its capability to provide maps of biophysical properties of adhered micro- and nanostructures at high spatial resolution (in the nanometre range), and in live conditions (buffers, cell media). In the biomedical community, these properties are much less explored than other type of characterization based on genetics and biochemistry, and they can be used to characterize physiological and pathological states, for early detection of diseases and to assess the in vivo behaviour of nanomaterials for drug delivery. In our lab, we aim at making the AFM as an integral part of the research in nanomedicine, increasing its throughput and introducing a user-friendly layout. Here we show some of the obtained results, from cell and tissue phenotyping (macrophages, cancer cell lines, primary fibroblasts, tissue sections), to the functional characterization of dynamically reconfigurable nanoparticles for drug delivery.

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Synthesis and Characterization of CoLi0.3Mn0.3Fe1.4O4 Ferrite Nanoparticles with Improved Saturation Magnetization Using Surfactant-Assisted Co-Precipitation

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Over the past two decades, there has been a notable increase in research focused on nanomaterials, particularly ferrite nanoparticles. Research interest in spinel ferrite magnetic nanoparticles has surged in recent years, driven by their potential applications in antennas, transformer, spintronics, biomedical fields, and catalysis. In our study, bare cobalt ferrite and Li+-Zn2+ co-doped cobalt ferrite nanoparticles (CoLi0.3Mn0.3Fe1.4O4) were synthesized using a co-precipitation approach both without surfactants and in the presence of three different surfactants, including cetyltrimethyl ammonium bromide (CTAB), polyvinyl pyrrolidone (PVP), and polyethylene glycol (PEG). The influence of various surfactants on the formation of crystal structure, morphology, magnetic and dielectric properties was investigated through X-ray diffraction (XRD), Scanning electron microscopy (SEM), vibrating sample magnetometer (VSM), and dielectric measurements. The XRD findings revealed the pure crystalline nature of synthesized samples with no impurity. The SEM micrographs revealed that sample coated with PVP is more uniform. The Energy Dispersive X-ray (EDX) analysis confirmed that the elemental composition was relevant with the expected values for the co-precipitation route. The type of surfactant used as a template influenced the magnetic properties of the synthesized cobalt ferrite nanoparticles by affecting their geometry. The presence of surfactants reduces the size of ferrite nanoparticles, leading to decreased coercivity and a significant enhancement in saturation magnetization, making it a suitable candidate for various applications. The dielectric loss of the synthesized nanoparticles significantly decreased, making the material suitable for high-frequency applications. The current findings indicate that the addition of various surfactants during sample preparation significantly controls the size of CoLi0.3Mn0.3Fe1.4O4 nanoparticles, which in turn has a noticeable impact on the magnetic properties of the material.

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Dynamics of photoactive colloids inside spherical microreactors

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Since the development of the first generation of self-propelled nanomotors, the field has undergone extensive exploration. A wide range of nanomotors has been synthesized, varying in materials, shapes, sizes, and propulsion mechanisms [1]. However, this diversity also introduces new challenges and raises fundamental questions, particularly regarding practical applications. Current research is primarily focused on areas such as drug delivery, pollutant degradation, sensing, and other fields that demand thorough investigation. These domains require comprehensive examinations of dynamics within confined spaces characterized by diverse obstacles and geometries, such as spheres, channels, and pores [2-4]. In this study, we analyzed the effects of confinement on the photocatalytic efficiency and collective motion behavior of different active colloids. As a result, this work introduces a novel "lab-in-a-drop"approach, which facilitates the exploration of new frontiers in understanding nanomotor behavior under confinement and in three-dimensional spaces, while advancing their potential applications in biomedicine, sensing, and environmental systems.

References

[1] He Zhao, Yuhong Zheng, Yuepeng Cai, Tailin Xu, Renfeng Dong, Xueji Zhang, Nano Today 52 (2023), 101939.
[2] Zuyao Xiao, Mengshi Wei, and Wei Wang, ACS Applied Materials & Interfaces, 11 (7) (2019), 6667-6684.
[3] Jiamin Ye, Yueyue Fan, Gaoli Niu, Baoli Zhou, Yong Kang, Xiaoyuan Ji, Nano Today 55 (2024), 102212.
[4] Tenjimbayashi, M., Mouterde, T., Roy, P. K., & Uto, K., Nanoscale 15 (47) (2023), 18980–18998.

Coffee Break / Poster Session (II) / 20

Multifunctional Copper-Cyclohexaphosphate Frameworks: Structural Insights, Electronic Properties, and DFT calculations

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Metal phosphates, a fascinating category of inorganic ring structures, have garnered considerable attention for their unique structural, physical, and chemical characteristics, including optical, electronic, and magnetic properties [1]. Cyclohexaphosphates, in particular, have attracted interest due to their high hydrolytic and thermal stabilities, as well as their strong complexation abilities [2]. Notably, metal cyclophosphate compounds display hierarchical structures with varying dimensionalities, including one-dimensional (1D) chains, two-dimensional (2D) layers, and complex three-dimensional (3D) frameworks. In this study, we report the synthesis and structural characterization of a new copper-cyclohexaphosphate compound, wherein the phosphoric anions and copper polyhedra are interconnected via Cu-O-P bonds, forming infinite ribbons of the formula. The crystal structure was elucidated using single-crystal X-ray diffraction (SCXRD). Infrared (IR) spectroscopy was employed to identify crucial functional groups and bonding interactions, while fluorescence measurements were carried out to investigate potential optical properties. Density functional theory (DFT) calculations were performed to gain greater insight of its electronic properties, revealing significant information about the HOMO-LUMO energy gap, nonlinear optical (NLO) properties, and quantum descriptors. The electronic density of states (DOS) was computed as well. Future investigations will aim to explore properties such as the magnetic behavior of the synthesized copper-cyclophosphate compound, potentially

offering valuable insights into its applications in multifunctional materials.
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Keywords

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Metal phosphates; copper-cyclohexaphosphate; X-ray diffraction; Hirshfeld surface; molecular orbital Theory, density of states (DOS).
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Reference

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[1] Rosario M. P. Colodrero, Pascual.Olivera-Pastor, Aurelio.Cabeza and Montse.Bazaga-García, Materials.,15(2022)1292.
[2] Samira.Sleymi, Massoud.Kahlaoui, Samiha.Dkhili, Salma.Besbes-Hentati, Sonia.Abid, Journal of Molecular Structure.,1127(2017) 175-182.

Coffee Break / Poster Session (III) / 21

METALBIO: METALES E IONES METÁLICOS EN SISTEMAS BIOLÓGICOS

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La red temática MetalBio, centrada en los metales e iones metálicos en sistemas biológicos, surge como evolución de la red creada en 2015, ampliando su alcance con la inclusión de nuevos grupos de investigación. Está compuesta por 13 grupos nacionales especializados en diversas áreas como la Química Bioinorgánica, los nanomateriales y los sistemas biológicos de interés terapéutico y ambiental.
Gracias a la consolidación de alianzas entre grupos, se han conseguido diseñar nanomateriales funcionalizados con propiedades teranósticas, así como estudiar sus interacciones con biomoléculas y sistemas biológicos. Además, gracias a la organización de proyectos colaborativos entre universidades se han desarrollado aplicaciones terapéuticas en modelos celulares y animales.

Por ello, este trabajo se centra en la preparación y modificación de nanopartículas con metalofármacos para su uso potencial como material teranóstico contra el cáncer. En este contexto, se ha funcionalizado una amplia variedad de sistemas basados en sílice con diferentes metalofármacos, que actúan como agentes citotóxicos y varios fluoróforos como isotiocianato de fluoresceína, Alexa Flúor o cumarinas e incluso compuestos con propiedades magnéticas, para dotar al material de capacidad de imagen y/o diagnóstico simultánea a su actividad terapéutica. Además, varios de los sistemas estudiados han utilizado varios fragmentos biológicos, como vitaminas y proteínas y otros agentes, para direccionar los sistemas y mejorar su selectividad contra las células cancerosas.
En esta comunicación se presentan los resultados más relevantes de MetalBio que abarcan el diseño síntesis y caracterización de los sistemas estudiados, así como su comportamiento como agentes terapéuticos o teranósticos *in vitro* e *in vivo*.

Coffee Break / Poster Session (III) / **22**

Ground State Degeneracy in Attractive Artificial Colloidal Ice with Frustrated Geometry

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We investigate the low energy state of an artificial colloidal ice, namely a collection of interacting paramagnetic colloids confined into a lattice of potential wells such that its geometry induces frustration via competing interactions at each vertex. In contrast to previous work with isotropic repulsions, we consider the case of time-average attractive interactions between the particles which are induced upon application of a high frequency, in-plane rotating magnetic field. We apply this new approach to the previously unstudied , geometrically frustrated penta-heptite lattice. Our numerical results reveal the degeneracy of the ground state resulting from the interplay between lattice geometry and pair interactions. The numerical procedure could be readily tested in experiments as it is based on real experimental parameters extracted from previous work.
The use of novel, frustrated geometry may be of interest for the fabrication of similar nano-scale logic device based on dipolar switching between the interacting units.

Coffee Break / Poster Session (II) / **23**

Advancements in Nanotechnology for Catalysis, Environmental Sustainability, and Next-Generation Memristors

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COMET-NANO leverages advances in nanotechnology to enhance catalysts at the nanoscale, essential in the chemical and environmental industries. The group develops hybrid nanosystems based

on silica, titania, carbon nanotubes, graphene oxide, magnetite, metallic nanoparticles, and bismuth-based materials, with improved catalytic and photocatalytic properties through green chemistry.
Success has been achieved in photocatalytic reactions, using different types of radiation, for the decomposition of organic contaminants in water, such as pharmaceuticals and dyes. Additionally, these materials are multifunctional, and capable of performing various coupling, oxidation, and polymerization reactions. With extensive experience in metallic complexes and nanostructured materials, we design advanced platforms for applications in the pharmaceutical, food, and petroleum industries and in environmental processes, improving both efficiency and sustainability.
The group also prepares different multifunctional platforms capable of capturing CO2 and N2, fixing them, and transforming them without the need to use multiple systems, employing starting materials with high surface-to-volume ratios and functionalizing them with specific organometallic complexes for the valorization of CO2 and N2. These versatile platforms will help reduce the greenhouse effect by decreasing CO2 concentrations, producing other carbon-based fuels, improving current energy efficiency through the photocatalytic reduction of CO2 to carbon monoxide or formic acid, and especially by transforming N2 to ammonia, a potential green fuel for energy production.
Recently, the COMET-NANO group has been granted a project to develop a new generation of cost-effective and high-performance memristors focused on leveraging 2D F-doped titanium dioxide materials to develop cost-effective and high-performance memristors. The unique properties of memristors, particularly their resistive switching behavior, make them suitable for in situ computing and integration into artificial synapse computing applications. The project builds on the successful synthesis of F-doped titanium dioxide nanoparticles from previous projects and extends this expertise to 2D materials, exploring hybrid systems with bismuth-based materials.

Coffee Break / Poster Session (II) / 24

Active chiral microswimmer: emergent behavior of suspensions mediated by hydrodynamic interaction

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The non-axisymmetric chiral squirmer [1], implemented within a Lattice Boltzmann code tailored for complex fluid dynamics [2], serves as a versatile tool to study the emergent behavior of microswimmer suspensions. Utilizing this model, we delve into the characterization of interactions between pairs of squirmers and explore their behavior in proximity to solid walls, as well as within the context of active chiral suspensions.
Our study encompasses a diverse spectrum of scenarios, ranging from individual interactions to more complex systems such as run-and-tumble dynamics, monolayers of rotors and rollers on walls, and beyond. By leveraging the capabilities of our computational framework, which solves the Stokes equations to accurately capture the hydrodynamics of active microswimmer suspensions, we gain insights into the intricate interplay of hydrodynamic forces, chirality, and confinement effects. Through systematic simulations and analysis, we elucidate the mechanisms governing the interaction dynamics between non-axisymmetric chiral squirmers, unveiling emergent collective behaviors and patterns. Moreover, we investigate the influence of solid interfaces on the motion and orientation of squirmers, providing valuable insights into boundary effects in active suspensions. Furthermore, our study extends to the realm of active chiral suspensions, where we explore the collective behavior and rheological properties of these systems. By characterizing the response of chiral squirmers to external stimuli and confinement, we contribute to a deeper understanding of the rich dynamics exhibited by active fluids. In summary, our research advances the understanding of non-axisymmetric chiral squirmers in complex fluid environments, offering valuable insights into their interactions, behavior near solid interfaces, and implications for active chiral suspensions. These findings pave the way for future studies aimed at harnessing and controlling the dynamics of active microswimmers for various applications in fields such as microfluidics, biomedicine, and soft robotics.

Coffee Break / Poster Session (III) / 25

Active Brownian Particles in Motility Landscapes

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Janus particles can be externally controlled in many different ways. The swim velocity of an active particle can be increased or decreased by tuning the light's power illumination, resulting in different self-assembly paths. This provides interesting applications, such as micro-motors where light–induced asymmetric velocity profiles give rise to directed motion.

While much is known about controlling Janus particles through static spatial motility landscapes, it still lacks a theoretical background. Moreover, the impact of spatio–temporal external fields as a way of controlling new assembly pathways remains unexplored.

In this work we provide theoretical framework for static motility patterns to more precisely characterize different assembly pathways in the dilute regime. Furthermore, we investigate the dynamical behaviour of active particles in response to an activity landscape, aiming to better understand the effects of spatio-temporal modulation of the self-propulsion velocity.

Coffee Break / Poster Session (II) / 26

Exploring the dynamics of elastic agents in ultrasound-driven fluids

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Ultrasound-guided drug and gene delivery offers a non-invasive, high-precision, low-toxicity method for the controlled and spatially precise delivery of drugs and macromolecules, encapsulated in microbubbles and submicron gas vesicles, to targeted areas such as cancer tumors. This technique significantly reduces the drug dose while improving therapeutic efficacy. In this study, we present a virtual environment where elastic objects function as contrast agents in ultrasound-mediated biomedical applications. We introduce a novel mesoscopic model that allows us to accurately investigate the rheological behavior of these agents and understand the nature of the ultrasound radiation forces acting on them, which is essential for optimizing ultrasound parameters. The computational model integrates molecular dynamics (MD) simulations, which track the dynamics of contrast agents, with computational fluid dynamics based on the Lattice Boltzmann (LB) method to resolve ultrasound-driven fluid interactions. In particular, we analyze the dynamics of microscale bubbles in complex fluids subjected to one-dimensional planar standing pressure waves. We explore the relationship between the pressure amplitude and the bubbles' compressibility, as well as the various interactions that arise due to ultrasound, paving the way for improved ultrasound-mediated drug and gene delivery systems.

Coffee Break / Poster Session (II) / 27

Collective Buoyancy-driven Dynamics in Swarming Enzymatic Nanomotors

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Enzymatic nanomotors harvest kinetic energy through the catalysis of chemical fuels. When a drop containing nanomotors is placed in a fuel-rich environment, they assemble into ordered groups and exhibit intriguing collective behaviour akin to the bioconvection of aerobic microorganismal suspensions. This collective behaviour presents numerous advantages compared to individual nanomotors, including expanded coverage and prolonged propulsion duration. However, the physical mechanisms underlying the collective motion have yet to be fully elucidated. Our study investigates the formation of enzymatic swarms using experimental analysis and computational modeling. We show that the directional movement of enzymatic nanomotor swarms is due to their solutal buoyancy. We investigate various factors that impact the movement of nanomotor swarms, such as particle concentration, fuel concentration, fuel viscosity, and vertical confinement. We examine the effects of these factors on swarm self-organization to gain a deeper understanding. In addition, the urease catalysis reaction produces ammonia and carbon dioxide, accelerating the directional movement of active swarms in urea compared with passive ones in the same conditions. The numerical analysis agrees with the experimental findings. Our findings are crucial for the potential biomedical applications of enzymatic nanomotor swarms, ranging from enhanced diffusion in bio-fluids and targeted delivery to cancer therapy.

Coffee Break / Poster Session (III) / 32

Universal Scaling of Clustering Instability for Interacting Active Brownian Particles

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Clustering is one of the mayor collective phenomena observed in active matter. We study the overdamped motion of interacting active Brownian particles in two dimensions. An instability in the pair correlation function causes the onset of clustering. This clustering mechanism depends mainly on the self-propulsion properties of the active particles and details of the interactions do not effect the scaling of the clustering instability. Theoretical predictions from repeated ring-kinetic theory are confirmed by agent-based simulations.

Invited Talks (IV) / 33

Synthetic Nano/Microrobots: Pioneering Solutions for Environmental and Biomedical Challenges

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Synthetic nano/microrobots have rapidly advanced, offering transformative capabilities in diverse fields through their autonomous movement, responsiveness to stimuli, and precise task execution at micro and nanoscale. This talk provides a brief introduction to the evolution of nano/microrobots, focusing on their breakthrough roles in environmental applications, such as pollutant detection, water purification, and energy harvesting, as well as their emerging potential in biomedical fields, including drug delivery and imaging. The presentation will then explore a series of works showcasing 2D-based robots, polymeric systems, and photocatalytic platforms, demonstrating their versatility across multiple domains. By leveraging innovative designs and materials, these nano/microrobots present a promising avenue for addressing critical global challenges in both environmental and medical landscapes.

Plenary Talks / 34

Photocatalytic Micromotors for Water Purification and Waste Valorization

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Photoactivated micro/nanomotors represent the next generation of self-propelled devices that can be easily actuated and controlled by using an external light source.1 Owing to their unique properties of photocatalytic-based systems —self-propelling as well as the generation of highly reactive radicals upon photoactivation—they have been widely explored for water cleaning and disinfection, wherein they have shown promising degradation rates.2,3 However, the selective oxidation of organic compounds remains a great technological challenge. Here, we introduce two strategies for enhancing the selective capture and oxidation of organic compounds based on surface modification by molecular polymer imprinting as well as magnetic actuation.4 The modified photocatalytic micromotors showed a selective oxidation of a specific pollutant from a complex liquid environment, resulting in higher pollutant removal rates compared to the unmodified ones. Moreover, the synergistic effect of combining optical and magnetic actuation for selectively generating phenol from benzene is also discussed.5 These approaches based on multifunctional photoresponsive micromotors hold promising applications in the fields of photocatalytic disinfection, water treatment, waste valorization and selective oxidation reactions.

References
[1] K. Villa, Chem. Commun. 59 (2023), 8375-8383, DOI:10.1039/D3CC01634J.
[2] K. Villa, et al. ACS Nano 13 (2019) 8135-8145, DOI:10.1021/acsnano.9b03184.
[3] X. Yuan, et al. Adv. Optical Mater. (2024), 2303137, DOI:10.1002/adom.202303137.
[4] X. Yuan, et al. Small 19 (2023), 2207303, DOI: 10.1002/smll.202207303.
[5] R. Ferrer et al. ACS Appl. Mater. Interfaces 2024, 16, 23, 30077–30087, DOI: 10.1021/acsami.4c03905.

Plenary Talks / 35

From large-scale functional porous materials to small-scale active platforms

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Controlling and understanding the mechanisms that govern crystallization processes is crucial in contemporary materials science, particularly in the field of reticular solids, where significant challenges remain. In this seminar, I will demonstrate how microfluidic synthetic conditions can control the size and shape of various functional porous crystals, such as metal-organic frameworks (MOFs) and covalent-organic frameworks (COFs). Specifically, I will show that microfluidic synthesis can produce the largest MOF single crystals with controlled nonequilibrium shapes reported to date, in contrast to the typical polyhedral microcrystals formed under bulk crystallization conditions. Additionally, I will illustrate how microfluidic technologies and confined synthesis can address several challenges in the COF research area. For instance, I will demonstrate that a confined synthesis can led to COFs with nanoscales sizes, enabling their processing and integration in active platforms. This is particularly significant given that COFs are typically obtained as powders with limited solubility and no melting point, making conventional processing techniques like solution processing or melt-extrusion inapplicable. The results to be presented will not only showcase the potential and versatility of MOFs and COFs but also demonstrate new avenues for their application in cutting-edge biotechnological solutions.

Plenary Talks / 36

From self-propelled micropumps to nanomotors

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Self-propelled micropumps are the immobilized version of nanomotors, sharing similar operational principles. Pumps offer valuable insights into the key parameters governing motion, with the added advantage of being easier to probe using various experimental techniques compared to their motile counterparts. In this talk, we will explore several examples demonstrating how micropumps can be used to understand, design, and optimize nanomotors. Particular attention will be given to ion-exchange-driven pumps and swimmers.
Ion exchange is one of the most interesting processes occurring at the interface between aqueous solutions and polymers endowed with sulfonic groups, such as the well-known Nafion1. When exchanged ions possess varying diffusion coefficients, this process generates local electric fields that can be utilized to propel fluid motion1,2. we demonstrate the design and fabrication of pumps and self-propelling micro/nanoswimmers based on Nafion, powered by ion exchange and fueled by salts. These Nafion micromachines are created through different lithographic techniques (colloidal, stencil, photo or electron beam lithographies) shaping Nafion into asymmetric structures3,4. The resulting micro/nanoswimmers exhibit fascinating collective motion in water driven by the interplay of their self-generated chemical/electric fields and their capability to pump surrounding matter towards them. The pumping activity of the micro/nanoswimmers induces the formation of growing mobile clusters, whose velocity increases with size. Such dynamic structures are able to trap nearby micro/nano-objects while purifying the liquid, which acts both as the transport media and as fuel3,4. This phenomenon holds promise for potential applications in water remediation currently under development.

References
[1]M. J. Esplandiu, D. Reguera, and J. Fraxedas, Soft Matter, 16 (2020) 3717.
[2]M. J. Esplandiu et al., Acc. Chem. Res., 51 (2018) 1921
[3]M. J. Esplandiu, D. Reguera, D. Romero-Guzman, A. M. Gallardo-Moreno, and J. Fraxedas, Nat. Commun. 13 (2022) 2812.
[4]J. Fraxedas, D. Reguera, M. J. Esplandiu, Faraday discussions, 249 (2024) 424.

Coffee Break / Poster Session (II) / 37

Exploring microfluidics for the microfabrication of blood clots

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The pursuit of enhanced drug testing for the treatment of diseases has led scientists to develop methodologies for delivering drugs into controlled and localized spaces. Blood-like substances have shown promise as noninvasive solutions [1]. Although individual blood cells have been investigated as drug carriers for various treatments, they face challenges in terms of drug release, targeting, and production. An alternative approach involves the use of blood clots as carrier entities by exploiting their natural formation process [2]. Recent studies have examined in vitro coagulation processes [3]. However, these investigations have neglected important factors, such as blood clot dimensions and composition, which are crucial for developing new controlled materials. Microfluidic mixing technologies enable mass transport governed solely by diffusion, allowing reactions to occur in a non-convective transport environment [4]. The application of these technologies permits the creation of products of various shapes and structures through controlled mixing [5]. In this study, we demonstrate a microfluidic method that effectively controls blood clot size and structure using a 5-inlet Y-junction-like device. Homogeneous and heterogeneous blood clots were constructed following our approach, highlighting the versatility of manufacturing clots using microfluidic approaches.
[1] S. Wang, et al. Med Drug Discov 13, (2022).
[2] H. Ceylan, et al. Sci Adv 7, 1 (2021).
[3] B. M. et al. Semin Cell Dev Biol 112, 1 (2021).
[4] A. G. Niculescu, et al. Nanomaterials 11, (2021).
[5] P. Martinez-Bulit, et al. Chemical Engineering Journal 435 (2022).

Invited Talk / 38

SELF-PROPULSION AT THE NANOSCALE: Exploiting Molecular Energy Relaxation Mechanisms

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Controlling the transport of micro and nano particles in liquids is a fundamental problem with the potential to revolutionize different emerging technologies [1]. The use of self-generated thermal gradients has been theoretically proposed and demonstrated in experiment to be a promising strategy to induce transport of microparticles in liquids [2]. Here we show that the anisotropic dissipation of excess molecular energy into the surrounding solvent can lead to the propulsion of nanoparticles [3]. We use all-atomic models of excited nanoparticles and of the solvent to investigate with molecular dynamics simulations the emergent particle propulsion as the excess energy is dissipated into the solvent. We report results in liquid water from: (i) nanoparticles functionalized with excited fluorophores [3]; (ii) high energy vibrationally excited molecules [4]. In both cases we find a marked energy flux anisotropy during relaxation which results in a temperature gradient across

the nanoparticle and in a net propulsion that leads to significant enhanced diffusion when periodic excitations are applied. In contrast to most models of self-phoresis, we find that propulsion occurs via short (⊠ 0.5ps) impulses. From our all-atomic description we identify the source of propulsion as a transient force imbalance with the surrounding solvent when hydrogen bonds are broken as a result of the prescribed molecular excitations. Finally, strategies to direct the motion of functionalized nanoparticles in a given direction using confined environments are also discussed.

References

[1] C. Bechinger, R. Di Leonardo, H. Löwen, C. Reichhardt, G. Volpe and G. Volpe, Rev. Mod. Phys. 88 (2016) 045006.
[2] H-R. Jiang, N. Yoshinaga and M. Sano, Phys. Rev. Lett. 105 (2010) 268302.
[3] C. Calero, E. L. Sibert III, R. Rey, Nanoscale 12 (2020) 7557.
[4] A. Jurado Romero, C. Calero, E. L. Sibert III, R. Rey, J. Chem. Phys. 158 (2023) 194501.

Plenary Talks (II) / **39**

Nanobots in nanomedicine

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Engineering medical nanomotors/nanobots will imply the use of biocompatible materials and biofriendly propulsion mechanisms. Our strategy comprises the use of biocatalysts such enzymes for converting biologically available fuels, such as the urea contained in the urine, into a propulsive force. Moreover, nanoparticles' chassis are generally recognized as safe (GRAS) material, FDA or EMA approved materials.
In my talk, I will present how we bioengineer hybrid nanobots combining the best from the two worlds: biology (enzymes) and (nano)technology (nano- micro-particles) providing swimming capabilities, biocompatibility, imaging, multifunctionality and actuation in vitro and in vivo. I will present some of the proof-of-concept applications of biocompatible nanobots such as the efficient transport of drugs into cancer cells and 3D spheroids (1), the imaging of swarms of nanobots in vivo in confined spaces like the bladder of living mice (2). Moreover, I will present our recent advances in the treatment of bladder cancer in mice using radionuclide-labelled nanobots (3) and crossing mucus layers present in the colon of mice (4).
References
[1] Hortelao et al. ACS Nano 2019, 13, (1), 429-439
[2] Hortelao et al. Sci. Robotics. 2021, 6, (52), eabd2823.
[3] C. Simó, M. Serra et al. Nat. Nanotech. 2024, 19, 554–564
[4] M. Serra et al. ACS Nano. 2024, 18, 16701-16714

Invited Talks (II) / **40**

Active emulsions formed by active particles in passive binary mixtures

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Systems containing active components are intrinsically out of equilibrium, while binary mixtures reach their equilibrium configuration when complete phase separation is achieved. Active particles

are found to stabilise non-equilibrium morphologies in phase separating binary mixtures by arresting coarsening, exerting active pressure that competes with surface tension driving forces. For moderate activities, an emulsion morphology is stabilised, where the droplet size is well-defined and controlled by activity. Conversely, the ability of active particles to drive phase-separated mixtures away from their equilibrium configuration is shown. A rich co-assembly behaviour is shown due to the competing energy scales involved in the system. In systems formed by droplets enclosing active particles, it is found that activity enhances shape fluctuations of the interface, matching recent experimental results using Quincke rollers. Furthermore, droplets containing polar active particles display active motion.

Invited Talks (II) / 41

Iridium Janus Nanomotor for Smart Drug Delivery

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In the last years, the use of nanomaterials in different fields has been continuously expanding due to their unique properties. Particularly, they play a crucial role as controlled drug delivery systems in medical applications. Among them, mesoporous silica nanoparticles are widely utilized due to their high loading capacity and ease of functionalization, enabling the incorporation of stimuli-responsive molecular gates for targeted and controlled drug release.

Nowadays, it is expected that nanomaterials not only control the drug released but also can move independently. Thus, new nanomaterials known as nanomotors are developed. In the present work, Janus nanoparticles have been employed to construct a nanomotor for controlled delivery. These nanomaterials are composed by two different nanoparticles: a mesoporous silica nanoparticle (MCM-41) provided with glucose oxidase and a boronic acid ester-based pH-sensitive gate-like ensemble, and iridium nanoparticles. Silica face allows encapsulation and further release of the drug while the iridium face causes the movement of the nanomotor. In the presence of glucose, the nanocarrier enzymatically produces gluconic acid and H2O2, causing pH decrease with consequent disassembly of the gating mechanism and release of the encapsulated cargo, whereas the catalytic decomposition of H2O2 on the iridium surface generates oxygen provoking the motion. This nanomotor was carefully characterized and successfully evaluate to on-command release of Doxorubicin in HeLa cancer cells. Then, we envision that the present results can open new opportunities for the construction of a large variety of nanomachines with self-propulsion capacity and enzymatic control for smart delivery of drugs.

Invited talks (II) / 42

Trying to control the collective behaviour of active particles

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Being groups of animals or populations of cells, active agents exhibit a fantastic richness of collective, or cooperative behaviour, responsible in many cases of providing function to biological or ecological systems. Can we develop predictive tools for these systems? Can we learn from them ways of fuctionalizing artificial materials? I'll address theses questions taking synthetic microswimmers as model systems, showing how one can tune their response to select different cooperative

states. I'll also stress how the understanding of simplified theoretical models, can help in predicting the collective behaviour of mixtures of self-propelled (Janus) colloids with different self-propulsion speeds.

Invited Talks (II) / **43**

Trying to control the collective behaviour of active particles

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Being groups of animals or populations of cells, active agents exhibit a fantastic richness of collective, or cooperative behaviour, responsible in many cases of providing function to biological or ecological systems. Can we develop predictive tools for these systems? Can we learn from them ways of fuctionalizing artificial materials? I'll address theses questions taking synthetic microswimmers as model systems, showing how one can tune their response to select different cooperative states. I'll also stress how the understanding of simplified theoretical models, can help in predicting the collective behaviour of mixtures of self-propelled (Janus) colloids with different self-propulsion speeds.

Plenary Talk (III) / **44**

Colloidal clusters and gels from active apolar colloids

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Active particles driven by a chemical reaction are the subject of intense research to date due to their rich physics, being intrinsically far from equilibrium, and their multiple technological applications [1]. Recent attention in the field is now shifting towards exploring the fascinating dynamics of mixture of active and passive systems. In this
talk, I will show different results obtained in my lab on investigating mixture of active and passive particles [2,3]. In particular, we have realized active colloidal rafts,composed of a single catalytic particle encircled by several shells of passive microspheres assembled via light activated, chemophoretic flow [3]. During growth, the rafts display self-propulsion with an average speed that decrease with the raft size. Brownian dynamics simulations that consider only the diffusiophoretic flow reproduce qualitatively the cluster kinetics but fail to explain the cluster propulsion mechanism. Using the Lorenz reciprocal theorem, propulsion emerges by considering hydrodynamics via the diffusiophoretic answer of the substrate to the generated chemophoretic flow.

[1] C. Bechinger, R. Di Leonardo, H. Löwen, C. Reichhardt, G. Volpe, and G. Volpe,
Rev. Mod. Phys. 88, 045006 (2016).
[2] H. Massana-Cid, J. Codina, I. Pagonabarraga, P. Tierno, Proc. Nat. acad. Sci. USA
115, 10618 (2018).
[3] D. Boniface, S. G. Leyva, I. Pagonabarraga, P. Tierno, Nature Communications 15,
5666 (2024).

Invited Talks (III) / **45**

Metal-organic framework based micromotors for biomedical applications

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Micromotors (MMs) are micro and nanoscale devices capable of converting energy into autonomous motion. Metal–organic frameworks (MOFs) are crystalline materials that display exceptional properties such as high porosity and biocompatibility. The combination of MOFs with MMs can result in a synergetic technology benefiting both from the enhanced fluid mixing of MMs and the exceptional properties of MOFs such as the capability for drug encapsulation. In this communication we will describe the synthesis of magnetocatalytic MOFs MMs using zeolitic imidazole organic frameworks as base units for modification with catalase for catalytic propulsion or ferrite nanoparticles for magnetic propulsion. We will also show the synthesis of Hong Kong University of Science and Technology (HKUST-1) MOFs using Cu/Ni/Pt MMs as nucleation spots by incubation with the specific ligand, benzene-1,3,5-tricarboxylic acid. Selected applications for Alzheimer biomarkers detection and controlled drug delivery will be briefly illustrated.

Invited Talks (III) / 46

Chemically fueled active vesicles for temporally controlled cargo release

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Chemical reactions in living systems are regulated by metabolic processes like the anabolic formation of bio-macromolecules and catabolic degradation of food into energy. These reactions often consume chemical energy and result in active self-assembled structures that exist under out-of-equilibrium (OOE) conditions, which facilitate unique functions of life. In specific, phospholipid molecules of cellular membranes are formed and sustained under OOE, which consume chemical energy to constantly form and breakdown the phospholipids. This provides unique properties like cellular plasticity, spatiotemporal control and regulate protein aggregation on cell surfaces.
In this talk, I will discuss a bio-inspired supramolecular system that forms transient lipid vesicle under OOE conditions, by consuming chemical energy, to result in vesicles with programmable lifetimes. We use simple imine chemistry for the formation of phospholipids and enzymatic ester hydrolysis for the degradation of lipids and the resultant vesicle. We will also demonstrate that the lifetime of these structures can be easily regulated based on the requirement. We are working towards using these active vesicles as an adaptive interface for targeted drug delivery.

Nanoinventum / 47

Programa nanoinventum: grans robots dissenyats per petits experts

Author: Jordi Díaz Marcos[1]

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Plenary Talk (IV) / 48

Defect lines morphology in three dimensional active nematics

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Within a living cell, motor proteins like kinesin are responsible of the transport of intracellular components. The functioning of this active transport is well known, and it has been employed to build synthetic assemblies of microtubules, which are stirred at the level of the single components and evolve out of thermal equilibrium. Such system is a paradigmatic example of an active material, and its realisation has originated lasting efforts, aimed to understand its crucial properties.
The presence of activity drives chaotic flow at the large scale and a sustained proliferation of topological defects, that retain some unique properties compared with passive liquid crystals. We use numerical simulations of a simple model of nematic liquid crystals in the presence of a microscopic active stress to study the morphology and dynamics of these topological defects to deduce fundamental properties of the turbulent state.
In a 3D periodic geometry, a statistically relevant wrapping component is present and quantitatively compatible with a phenomenon of defects percolation. Moreover, while the linear size of finite defects scales linearly with active length, it verifies an inverse quadratic dependence for wrapping defects. The shorter is the active length scale, the more times the defect lines wrap around the periodic boundaries, resulting in extremely long and tangled structures.

Plenary Talk (IV) / 49

Active nematic defects

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This talk will discuss recent results pertaining to 2D active nematics in flat space. We will focus on defect number fluctuations and how they relate to the system structure and overall correlations. Contrary to what is often found in active matter, we do not observe giant number fluctuations. Instead, we find that the system of defects exhibits hyperuniformity.

Plenary Talk (IV) / 50

Microfluidic transport of colloidal particles and solitons in liquid crystals

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The controlled transport and assembly of colloidal cargo within confined micro-environments is a challenging endeavor with significant implications for both technological applications and fundamental science. To achieve directed motion, both self-propelled and externally driven colloidal particles and droplets must be guided by breaking fore-aft symmetry in a controlled manner. Liquid

crystals offer a promising approach for this purpose due to their intrinsic anisotropy and the ability to manipulate their orientation using external electromagnetic fields.

In this presentation, I will discuss our experiments where non-spherical colloidal particles are propelled in a nematic liquid crystal layer using alternating electric fields, while we control their direction of motion and clustering with a permanent magnetic field. Additionally, this approach can be applied to propel and steer stable solitons, known as spherulites or "baby-skyrmions." These structures can be reversibly generated within the liquid crystal layer, acting as colloidal quasiparticles with complex interactions and transport modes, demonstrating their potential to carry passive colloidal cargo effectively.

Invited Talks (IV) / 51

Motion-Enhanced Enantiobiorecognition Events using Micromachines with Implanted (Supra)Molecular Chirality

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Chiral enantiomers have identical chemical formula, molecular weight and physicochemical properties except for optical rotation, whereas they exhibit different biological and pharmacological properties. Many biologically active substances, such as amino acids, proteins, enzymes, DNA, etc., are chiral. While only one enantiomer of a chiral drug, usually the L–form, exhibits useful therapeutic effects, the D–form may generate adverse reaction to living organisms [1]. Therefore, it is crucial to develop simple, effective and generic analytical methods for chiral separation and screening of pharmaceutical intermediates and active pharmaceutical ingredients (APIs). In this line, the combination of micromachines with chirality might offer an innovative pathway to enhance the detection and discrimination of enantiobiorecognition events ad hoc by taking advantage of their inherent motion activity.
Herein, a novel multifunctional micromachine is presented to elucidate the concept of 'enantiorecognition-on-the-fly'. The multifunctional micromachine architecture simultaneously exhibits i) chiral, ii) magnetic, and iii) fluorescent properties in combination with iv) self-propulsion [2]. Using Surface Engineering, the enantiobiorecognition features were robustly integrated by anchoring a chiral supramolecular host moiety as β-cyclodextrin (β-CD), which successfully demonstrated its suitability to accommodate chiral biomolecules (i.e., amino acids) with different binding kinetics via supramolecular host–guest encapsulation. Our findings demonstrate that motion outperform static systems in terms of enantiodiscrmination ability.

References
[1] J. Muñoz, A. González-Campo, M. Riba, et al. "Chiral magnetic-nonobiofluids for rapid electrochemical screening of enantiomers at a magneto nanocomposie graphene-paste electrode". Biosensors and Bioelectronics (2018), 105, 95-102.
[2] J. Muñoz, M. Urso, M. Pumera. "Self-Propelled Multifunctional Microrobots Harboring Chiral Supramolecular Selectors for 'Enantiorecognition-on-the-Fly'". Angewandte Chemie (2022), 61, e202116090.

Invited Talks (V) / 52

Optimizing Microscopy Setups for Active Matter Studies: Insights and Solutions from Zeiss

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Invited Talks (V) / 53

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Plenary Talks (II) / 55

Sperm-driven micromotors moving in complex environments and their potential biomedical applications

Author: Mariana Medina-Sanchez[1]

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Several concepts have been pursued by different research groups worldwide to realize untethered propulsion on a small size scale. Potential geometries for such untethered devices range from tubular microjets, Janus particles, or rods, over bio-inspired artificial flagella, to helical micromotors. Physical micromotors and microrobots for example are based on external physical fields such as magnetic fields and ultrasound, while the bio-hybrid micromotors mainly rely on the propulsion ability of the coupled biological entity (e.g. sperm, bacteria). In particular, I am going to talk about sperm-hybrid microrobots designed to increase the pregnancy success rate and reduce the invasiveness of current assisted fertilization technologies. These sperm-hybrid microrobots have also been used as drug carriers for gynecological cancer treatment. Finally, to translate these technologies to pre-clinical trials, we have recently reported the successful tracking of magnetically-driven micromotors in phantom, ex-vivo, and living mice with high spatial and temporal resolution employing photoacoustic imaging

Pitch Presentations / 56

Modulation of Amyloid-β Aggregation with Metal Nanoparticles

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Conformational pathologies, including neurodegenerative ones, are characterized by misfolded proteins called amyloids, which lose their physiological role and acquire toxicity. The accumulation and spread of amyloids is related to an impaired proteostasis network. Chaperones, as key actors of proteostasis, have thus become promising drug targets and models.
We are exploring how metal nanoparticles might be used to either emulate or assist natural chaperones' action against amyloid accumulation in Alzheimer's disease.

Pitch Presentations / 57

Hydrodynamic viscous levitation of magnetically driven S-shape propellers

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Hydrodynamic interactions (HIs), namely solvent-mediated long-range interactions between dispersed, microscopic particles, play a crucial role in the emergent dynamics of many active systems, from swimming bacteria to swarms of propelling microrobots. For example, HIs forces the bacteria E. Coli tend to swim close to a surface, where it performs a circular trajectory nearby. The attraction results from the pusher type force dipole of the bacteria, which creates a flow field able to force the bacteria towards the wall. Similarly, for a puller type swimmer, the generated flow field induces a repulsion from the wall. However, for pullers, the alignment parallel to the wall is not a stable configuration. Inspired by this effect, we design a microscale magnetic rotor able to produce a puller-like force dipole, but with a stable alignment parallel to the wall.

These S-shape lithographic particles are doped with nanoscale magnetic colloids and can be manipulated via external, time-dependent magnetic fields. Under a rotating, circularly polarized magnetic field, these propellers are subjected to a magnetic torque, and rotate exerting a force on the surrounding fluid. Because of the anisotropy of the drag coefficient on the elongated shape, similar to a pusher type bacterium, a pair of forces arise pointing towards the center of mass of the particle. Since the S-shape rotates above a wall, it experiences an upward lift force. We optimize the shape of the S particle to maximize the lift force. Since the lift force decreases with the distance from the wall, we calculate the equilibrium rotation height for different rotation frequencies. We find that an S-shaped particle with the cross-section radius of 3 microns and the length of 120 microns lifts to a height of around 100 microns when rotated at a frequency of 6 Hz in water-glycerol mixture with the viscosity 9.7 mPa s.

Pitch Presentations / **58**

Growing and Shaping Metal–Organic Framework Single Crystals at the Millimeter Scale

Authors: Alessandro Sorrenti[1]; Josep Puigmarti Luis[1]; Maria Guix[1]; Thao Nguyen[1]

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Morphological control of crystals is utterly important in reticular chemistry, especially as a fundamental strategy toward preparing functional materials of superior properties. Despite the notable advancements in the realm of metal-organic frameworks (MOFs), where endeavors primarily focus on shape manipulation at the nano- and microscale during bulk synthesis and subsequent processing at the mesoscale (e.g., incorporation into polycrystalline films, patterns, and composites), a notable challenge persists in attaining a meticulous control over both the shape and size of macroscopic single crystals.
Here we successfully demonstrated the spatial and morphological control of crystal growth at the millimeter scale from a non-equilibrium state through the utilization of a microfluidic device. Specifically, we employed PDMS channels to confine CuGHG, a peptide-based MOF, where crystal formation occurred as a consequence of a diffusion-controlled supply of precursors within an advection-free microenvironment. Depending on the concentration of the feeding solution, continuous growth or shrinkage of the crystals was observed and recorded by time-lapse microscope. Our method not only introduces a novel approach for precisely shaping large-scale single crystals from metastable solutions but also draws attention to its intriguing resemblance to two fundamental morphogenesis strategies observed in biomineralization. The presented results, therefore, establish a fundamental basis for future studies in materials science, shedding light on how the size and shape of artificial crystals can intricately influence their properties and functions.Moreover, our findings provide a strategic avenue for tailoring the size and shape of peptide-based MOF single crystals to specific applications. This approach not only expands the horizons of crystal engineering but also opens up possibilities for the design and customization of materials with desired properties for various technological applications.

Pitch Presentations / 59

Magnetic (nano)actuators for enhanced mass transfer in voltammetric and spectroelectrochemical assays.

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Emerging Contaminants (ECs) are considered anthropogenic impact indicators, whose detection and quantification contribute to understanding their occurrence, distribution, and potential toxicity, allowing for effective mitigation strategies and environmental management. Electrochemical sensors based on screen-printed electrodes (SPE) have gained significant attention due to their advantages such as fast response, simplicity, sensitivity, cost-effectiveness and tuneability. In this sense, progress in nanomaterials preparation and modification strategies of SPEs leads to improved sensitivity and specificity, making these systems suitable for voltammetric detecting a wide range of ECs.
Other electrochemical methods to screen analytes and processes are Spectroelectrochemical (SEC) measurements in the UV-vis region. These are based on the changes that occur in the absorption spectrum of a liquid sample when an electrochemical process consumes or generates an absorbing species at the working electrode. In normal reflection mode, these measurements are less sensitive than those obtained in parallel configuration. This is because the monitored sample volume contains a much smaller diffusion layer created by the electrochemical processes, i.e. the region where the relevant optical changes take place. On the other hand, the standard configuration is more robust and reproducible and, currently, it is the only one commercially available.
In some cases, parameters such as repeatability, reproducibility and sensitivity seemed to be improved by the incorporation of magnetic cobalt ferrite nanoparticles into the measuring solution, acting as diffusion enhancers at the nanometric range.
This work describes a strategy to improve normal measurements in voltammetric and SEC analysis, The strategy is based on the addition of magnetic cobalt ferrite nanoparticles (MNPs) The induced movement of the MNPs (nano-enabled stirring) enhances the transport of matter to and from the electrode, producing a rapid renewal of the diffusion layer and, therefore, an increase in current signal.

Pitch Presentations / 60

NEW INSIGHTS INTO SELF–PHORESIS

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Chemophoresis describes the displacement of a particle in an ambient fluid due to a gradient in chemical composition. Classic phoresis can be understood through linear-response theory: in the presence of a sufficiently small, externally imposed gradient $(\nabla n)_{\rm ext}$ in concentration, the phoretic velocity of the particle is $\mathbf{V} = \mathcal{L}_{\rm lin}(\nabla n)_{\rm ext}$, in terms of the phoretic coefficient $\mathcal{L}_{\rm lin}$ given by a Green-Kubo expression.

Self-phoretic particles induce a composition gradient $(\nabla n)_{\rm act}$ through catalytic activity and provide a physical realization of artificial swimmers. Experimental observations are then customarily addressed as another instance of classic phoresis, $\mathbf{V} = \mathcal{L}_{\rm lin}(\nabla n)_{\rm act}$.

However, an additional role of the particle's chemical activity has been recently identified as responsible for a specific activity-induced response $\mathcal{L}_{\rm act}$, so that one has to write $\mathbf{V} = (\mathcal{L}_{\rm lin} + \mathcal{L}_{\rm act})\,[(\nabla n)_{\rm ext} + (\nabla n)_{\rm act}]$ in the more general scenario. This means a change in paradigm as it disproves the claim that "self-phoresis is phoresis in a self-induced gradient".

- A. Domínguez, M.N. Popescu, C. Rohwer, S. Dietrich, *Phys. Rev. Lett.* **125**, 268002 (2020).
- A. Domínguez, M.N. Popescu, *Curr. Op. Coll. & Interface Sci.*, **61**, 101610 (2022).
- A. Domínguez, M.N. Popescu, *Mol. Phys.*, doi: 10.1080/00268976.2024.2396545 (2024).
- A. Domínguez, M.N. Popescu, *arXiv:2404.16435*
- A. Domínguez, M.N. Popescu, *arXiv:2407.08314*

Pitch Presentations (II) / **61**

MOTION AND CONTROL OF VIRTUAL PARTICLES IN CONFINED CHIRAL LIQUID CRYSTALS

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Cholesteric phases are liquid crystals in which a helical twist can be induced by the presence of a chiral agent. This twist, with a periodicity or pitch (p), can be frustrated under geometrical confinement comparable to p. Under those conditions, skyrmions can be formed if the material undergoes an instability. Skyrmions are topologically protected solitonic-like structures [1-3], formed by the spatial discordance in the orientation of the molecules of the liquid crystal, forming a torus in which the principal axis of the molecules turns 180o. Skyrmions behave as quasi-particles and can be driven by the action of a modulated AC electric field [1-3]. However, the directionality of their motion has, so far, only been in-situ controlled using complex optical systems [3]. In our work, we study the propulsion of skyrmions under modulated AC electric fields of different amplitude, carrier, and modulation frequencies. We also demonstrate the capability of an external fixed magnetic field to steer driven skyrmions, which can be inserted and controlled within microfluidic channels. Experimental suggest an acceleration when skyrmions are introduced in micro-channels due to distortions in the LC molecular alignment generated by the presence of homeotropic walls. We also show that skyrmions can act as micro-cargo transporters.

[1] Shon, et. al., Nat. Commun, 10:14744 (2019), 1-11.
[2] Ackerman, et. al., Nat. Commun, 6:673 (2017), 1-13.
[3] Shon, et. al., Opt. Express, 28:5 (2020), 6306-6319.

Pitch Presentations (II) / **62**

Fuel Driven Dynamic Phospholipid Vesicles with Programmable Lifetime for Controlled Cargo Release

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Metabolic processes are crucial for sustaining life, involving the cyclic synthesis (anabolism) and degradation (catabolism) of chemical and supramolecular structures through the expense of chemical

energy [1]. These highly dynamic structures which form under out-of-equilibrium (OOE) conditions define the hallmark features of life such as adaptivity and spatiotemporal control [2]. At the cellular level, metabolic activities govern functions by modulating phospholipid synthesis and breakdown. However, replicating synthetic vesicles that mimic cellular phospholipid membranes has proven difficult. In this work, we present a bioinspired approach for the in situ synthesis of biomimetic phospholipids and their self-assembly, driven by chemical fuel under physiological conditions, resulting in vesicles with a controllable lifetime. The phospholipids are formed via an amino-ester bond through imine formation (anabolic reaction), leading to spontaneous vesicle formation. In the presence of lipase, the ester bond is hydrolysed (catabolic reaction), triggering vesicle disassembly. Spectroscopic and microscopic analysis confirmed the continuous cycle of vesicle formation and breakdown. By varying lipase concentrations, we fine-tuned the vesicles'lifetimes, ranging from minutes to hours. Additionally, by supplying excess fuel, we sustained these dynamic vesicles in its assembly state. Detailed studies showed that the assembly can be temporally controlled by the amount of fuel supplied as well as the kinetics of the enzymatic reaction. We also demonstrated the potential application of these vesicles for drug release by encapsulating hydrophobic and hydrophilic model drugs and showed that the release kinetics of the encapsulated cargo molecules can be dynamically regulated for potential applications in adaptive nanomedicine.

Pitch Presentations (II) / 63

Active chiral microswimmer: emergent behavior of suspensions mediated by hydrodynamic interaction

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The non-axisymmetric chiral squirmer [1], implemented within a Lattice Boltzmann code tailored for complex fluid dynamics [2], serves as a versatile tool to study the emergent behavior of microswimmer suspensions. Utilizing this model, we delve into the characterization of interactions between pairs of squirmers and explore their behavior in proximity to solid walls, as well as within the context of active chiral suspensions.
Our study encompasses a diverse spectrum of scenarios, ranging from individual interactions to more complex systems such as run-and-tumble dynamics, monolayers of rotors and rollers on walls, and beyond. By leveraging the capabilities of our computational framework, which solves the Stokes equations to accurately capture the hydrodynamics of active microswimmer suspensions, we gain insights into the intricate interplay of hydrodynamic forces, chirality, and confinement effects. Through systematic simulations and analysis, we elucidate the mechanisms governing the interaction dynamics between non-axisymmetric chiral squirmers, unveiling emergent collective behaviors and patterns. Moreover, we investigate the influence of solid interfaces on the motion and orientation of squirmers, providing valuable insights into boundary effects in active suspensions. Furthermore, our study extends to the realm of active chiral suspensions, where we explore the collective behavior and rheological properties of these systems. By characterizing the response of chiral squirmers to external stimuli and confinement, we contribute to a deeper understanding of the rich dynamics exhibited by active fluids. In summary, our research advances the understanding of non-axisymmetric chiral squirmers in complex fluid environments, offering valuable insights into their interactions, behavior near solid interfaces, and implications for active chiral suspensions. These findings pave the way for future studies aimed at harnessing and controlling the dynamics of active microswimmers for various applications in fields such as microfluidics, biomedicine, and soft robotics.

Pitch Presentations (II) / 64

Collective Buoyancy-driven Dynamics in Swarming Enzymatic Nanomotors

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Enzymatic nanomotors harvest kinetic energy through the catalysis of chemical fuels. When a drop containing nanomotors is placed in a fuel-rich environment, they assemble into ordered groups and exhibit intriguing collective behaviour akin to the bioconvection of aerobic microorganismal suspensions. This collective behaviour presents numerous advantages compared to individual nanomotors, including expanded coverage and prolonged propulsion duration. However, the physical mechanisms underlying the collective motion have yet to be fully elucidated. Our study investigates the formation of enzymatic swarms using experimental analysis and computational modeling. We show that the directional movement of enzymatic nanomotor swarms is due to their solutal buoyancy. We investigate various factors that impact the movement of nanomotor swarms, such as particle concentration, fuel concentration, fuel viscosity, and vertical confinement. We examine the effects of these factors on swarm self-organization to gain a deeper understanding. In addition, the urease catalysis reaction produces ammonia and carbon dioxide, accelerating the directional movement of active swarms in urea compared with passive ones in the same conditions. The numerical analysis agrees with the experimental findings. Our findings are crucial for the potential biomedical applications of enzymatic nanomotor swarms, ranging from enhanced diffusion in bio-fluids and targeted delivery to cancer therapy.

Pitch Presentations (II) / 65

Exploring microfluidics for the microfabrication of blood clots

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The pursuit of enhanced drug testing for the treatment of diseases has led scientists to develop methodologies for delivering drugs into controlled and localized spaces. Blood-like substances have shown promise as noninvasive solutions [1]. Although individual blood cells have been investigated as drug carriers for various treatments, they face challenges in terms of drug release, targeting, and production. An alternative approach involves the use of blood clots as carrier entities by exploiting their natural formation process [2]. Recent studies have examined in vitro coagulation processes [3]. However, these investigations have neglected important factors, such as blood clot dimensions and composition, which are crucial for developing new controlled materials. Microfluidic mixing technologies enable mass transport governed solely by diffusion, allowing reactions to occur in a non-convective transport environment [4]. The application of these technologies permits the creation of products of various shapes and structures through controlled mixing [5]. In this study, we demonstrate a microfluidic method that effectively controls blood clot size and structure using a 5-inlet Y-junction-like device. Homogeneous and heterogeneous blood clots were constructed following our approach, highlighting the versatility of manufacturing clots using microfluidic approaches.
[1] S. Wang, et al. Med Drug Discov 13, (2022).
[2] H. Ceylan, et al. Sci Adv 7, 1 (2021).
[3] B. M. et al. Semin Cell Dev Biol 112, 1 (2021).
[4] A. G. Niculescu, et al. Nanomaterials 11, (2021).
[5] P. Martinez-Bulit, et al. Chemical Engineering Journal 435 (2022).

Pitch Presentations (III) / 66

Integrating AFM in Nanomedicine: Biophysical Mapping for Diagnostics and Drug Delivery

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The atomic force microscope (AFM) is gaining progressive attention for its capability to provide maps of biophysical properties of adhered micro- and nanostructures at high spatial resolution (in the nanometre range), and in live conditions (buffers, cell media). In the biomedical community, these properties are much less explored than other type of characterization based on genetics and biochemistry, and they can be used to characterize physiological and pathological states, for early detection of diseases and to assess the in vivo behaviour of nanomaterials for drug delivery. In our lab, we aim at making the AFM as an integral part of the research in nanomedicine, increasing its throughput and introducing a user-friendly layout. Here we show some of the obtained results, from cell and tissue phenotyping (macrophages, cancer cell lines, primary fibroblasts, tissue sections), to the functional characterization of dynamically reconfigurable nanoparticles for drug delivery.

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Emergence of a vortex lattice in anisotropic active flow under confinement

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We assemble a biomimetic active material from microscopic components like cells' filaments and protein motors that consume energy and generate continuous motion. Such active systems are capable of self-organization at different length and time scales, often exhibiting turbulent flows and the emergence of long-range orientational order, which is a characteristic of active nematics (AN). Previously, it was demonstrated that, by bringing into contact a two-dimensional AN with an anisotropic oil that features smectic liquid-crystalline order, it is possible to transform the originally turbulent flow of the active fluid into well-aligned flows ordered by a magnetic field [1]. Alternatively, the flow of active nematic could be controlled by confining walls [2] or arrangements of obstacles [3].
n present work we combine both approaches: well-aligned flows of AN ordered by a magnetic field were confined between walls of PDMS channels. The resulting quasi-laminar flows of AN are perturbed by closely located channel walls and reorganized in arrays of vortexes forming an hexagonal lattice. The emergence of vortex lattices is correlated with positional ordering of topological defects and the appearance of density patterns. The observed self-organization of the active flows is activity dependent and reflects the inherent properties of the aligned AN. The described system is an example of pattern formation from instabilities of AN flows and suggests potential applications in the design and control of active materials.

[1] P. Guillamat, et al., Proc. Natl. Acad. Sci. U. S. A., 113, 20 (2016).
[2] J.Hardoüin et al., Soft Matter, 16, (2020).
[3] B. Zhang, et al., Phys. Rev. Research, 2, 4 (2020).

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Dynamics of photoactive colloids inside spherical microreactors

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Since the development of the first generation of self-propelled nanomotors, the field has undergone extensive exploration. A wide range of nanomotors has been synthesized, varying in materials, shapes, sizes, and propulsion mechanisms [1]. However, this diversity also introduces new challenges and raises fundamental questions, particularly regarding practical applications. Current research is primarily focused on areas such as drug delivery, pollutant degradation, sensing, and other fields that demand thorough investigation. These domains require comprehensive examinations of dynamics within confined spaces characterized by diverse obstacles and geometries, such as spheres, channels, and pores [2-4]. In this study, we analyzed the effects of confinement on the photocatalytic efficiency and collective motion behavior of different active colloids. As a result, this work introduces a novel "lab-in-a-drop"approach, which facilitates the exploration of new frontiers in understanding nanomotor behavior under confinement and in three-dimensional spaces, while advancing their potential applications in biomedicine, sensing, and environmental systems.

References

[1] He Zhao, Yuhong Zheng, Yuepeng Cai, Tailin Xu, Renfeng Dong, Xueji Zhang, Nano Today 52 (2023), 101939.
[2] Zuyao Xiao, Mengshi Wei, and Wei Wang, ACS Applied Materials & Interfaces, 11 (7) (2019), 6667-6684.
[3] Jiamin Ye, Yueyue Fan, Gaoli Niu, Baoli Zhou, Yong Kang, Xiaoyuan Ji, Nano Today 55 (2024), 102212.
[4] Tenjimbayashi, M., Mouterde, T., Roy, P. K., & Uto, K., Nanoscale 15 (47) (2023), 18980–18998.

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Ground State Degeneracy in Attractive Artificial Colloidal Ice with Frustrated Geometry

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We investigate the low energy state of an artificial colloidal ice, namely a collection of interacting paramagnetic colloids confined into a lattice of potential wells such that its geometry induces frustration via competing interactions at each vertex. In contrast to previous work with isotropic repulsions, we consider the case of time-average attractive interactions between the particles which are induced upon application of a high frequency, in-plane rotating magnetic field. We apply this new approach to the previously unstudied , geometrically frustrated penta-heptite lattice. Our numerical results reveal the degeneracy of the ground state resulting from the interplay between lattice geometry and pair interactions. The numerical procedure could be readily tested in experiments as it is based on real experimental parameters extracted from previous work.
The use of novel, frustrated geometry may be of interest for the fabrication of similar nano-scale logic device based on dipolar switching between the interacting units.

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Universal Scaling of Clustering Instability for Interacting Active Brownian Particles

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Clustering is one of the mayor collective phenomena observed in active matter. We study the overdamped motion of interacting active Brownian particles in two dimensions. An instability in the pair correlation function causes the onset of clustering. This clustering mechanism depends mainly on the self-propulsion properties of the active particles and details of the interactions do not effect the scaling of the clustering instability. Theoretical predictions from repeated ring-kinetic theory are confirmed by agent-based simulations.