様　式　Ｃ－１９、Ｆ－１９－１、Ｚ－１９　（共通）

# 科学研究費助成事業　　研究成果報告書

令和　５ 年　 ６ 月　 ８ 日現在

機関番号：１４３０１
研究種目：基盤研究(C)（一般）
研究期間：2020～2022
課題番号：２０Ｋ０３７８６

研究課題名（和文）Metallo-Dielectric Janus Particles as Building Blocks for Designer Active Materials

研究課題名（英文）Metallo-Dielectric Janus Particles as Building Blocks for Designer Active Materials

研究代表者
ＭＯＬＩＮＡ　ＪＯＨＮ（Molina, John）

京都大学・工学研究科・助教

研究者番号：２０７２７５８１

交付決定額（研究期間全体）：（直接経費）　　2,800,000円

研究成果の概要（和文）：本研究の目的は、単粒子・多粒子アクティブ・コロイドのダイナミクスのメカニズムを理解することである。そのために、交流・直流電場下でのコロイド粒子の電気流体力学と剛体力学を考慮した計算手法を開発した。その結果、金属・誘電体ヤヌス粒子のダイナミクスを再現することに成功し、電場強度に対する速度依存性や粒子表面付近の強い電場勾配に伴う高周波での速度反転を再現した。さらに、直流電場下での誘電体粒子の集団ダイナミクスを調べ、流体力学と静電気力学の相互作用が実験で観察された異なる相をどのように説明するかを明らかにしました。最後に、複雑な流れの構成関係やストークス流問題の解を推測できる機械学習法を開発しました。

研究成果の学術的意義や社会的意義
We have developed physical models that can be used to understand the rich dynamics of active colloidal particles, which can be used as building blocks for novel materials. We have also developed Machine-Learning methods that can significantly enhance our ability to predict complex flows.

研究成果の概要（英文）：The purpose of this work is to understand the mechanisms behind the rich single- and many-particle dynamics of active colloids. For this, we have developed a computational method that accounts for the electro-hydrodynamics and rigid-body dynamics of colloidal particles under AC/DC fields. We succeeded in reproducing the dynamics of metallo-dielectric Janus particles, including the velocity dependence on the electric field strength, as well as the velocity reversal at high frequencies, which are accompanied by strong field gradients near the particle surface. We have further investigated the collective dynamics of dielectric particles under DC fields, to reveal how the interplay between the hydrodynamics and electrostatics accounts for the different phases observed experimentally. Finally, we have developed Machine-Learning methods capable of inferring constitutive relations for complex flows, as well as solutions to Stokes flow problems.

研究分野：Computational Soft Matter Physics

キーワード：Electro-Hydrodynamics　Active Particles　Electrophoresis　Janus Particles　Quincke Rollers　Machine Learning　Multi-Scale Simulations　Flow Inference

様　式　Ｃ－１９、Ｆ－１９－１、Ｚ－１９（共通）

１．研究開始当初の背景

Active systems, composed of “agents” capable of consuming energy to perform work (e.g., self-propulsion), are ubiquitous in nature (e.g., molecular motors, bacteria, spermatozoa). From a fundamental point of view, the fact that these active agents are continuously injecting/dissipating energy means that they constitute an inherently out-of-equilibrium system. Thus, it is not surprising that these active soft matter systems have quickly become the ideal testbed to develop theories of non-equilibrium physics. As biological realizations of active soft matter can be incredibly complex to study, both experimentally and theoretically, much attention has been given to developing synthetic active particles (Abbot and Velev, COCIS **21**, 1-3, 2016), which also offer interesting technological applications (e.g., targeted cargo transport). These active particles can be built to convert local thermal, chemical, or electro-magnetic energy into work, typically through self-phoresis, that is, by self-generating a localized gradient in a suitable field.

Among the various realization of synthetic active matter, two examples have quickly become the benchmark experimental systems: (1) Metallo-dielectric Janus particles and (2) Quincke rollers dispersed in electrolyte solutions. In both cases, the particles are powered by external (AC or DC) electric fields, i.e., they are fuel-free. This makes them particularly well suited for bio-medical applications. We note that even though the energy comes from an external source, these particles still behave as active particles, as they move along independent paths (the direction of motion is not necessary dictated by the external field). In the case of (1) metallo-dielectric Janus Particles, composed of two halves with distinct material properties (i.e., permittivity and/or conductivity), the physical mechanism behind the self-propulsion, at least in the simplest case, is known as Induced-Charge Electrophoresis (ICEP), originally proposed by Bazan and Squires (PRL **92**, 066101, 2004). Under ICEP, a Janus particle in an external AC/DC field becomes asymmetrically polarized (due to the asymmetric material properties), with a larger induced surface charge on the metal hemisphere, leading to a stronger electro-hydrodynamic flow, which in turns leads to a net propulsion in the direction of the dielectric hemisphere. In the case of (2) Quincke rollers, dielectric particles are made to rotate under a DC electric field thanks to the Quincke effect. This Quincke mechanism arises from the rotation of the dielectric particle due a spontaneous symmetry breaking of the induced surface charges. In the presence of a wall, this rotation leads to a translation of the particle.

These active matter systems have been shown experimentally to exhibit very complex single particle and collective motions (Yan et al., Nat. Mater. **15**, 1095, 2016; Karani et al., PRL **123**, 208002, 2019), a detailed understanding of which is still lacking. The issue lies in the complex electro-hydrodynamic coupling between these active particles and their environment, as well as with each other. Note, for example, that standard ICEP theory (Boymelgreen and Miloh, Electrophoresis **33**, 870, 2012) can explain the motion of single Janus particles at low frequency, which move with the dielectric side forward, but not the motion at high-frequencies, where experiments have shown a velocity-reversal, with the particles moving with the metal side forward (Boymelgreen et al., Langmuir **32**, 9540, 2016).

Such systems have typically been studied using numerical simulations, however, most studies of active systems employ models that are overly simplified, which makes direct comparisons to experiments a non-trivial task. This is further amplified by the fact that the experiments themselves are usually not fully characterized. For example, the full 3D flow field generated by the swimmers cannot be measured directly and/or the boundary conditions at the particle surface might be unknown.

２．研究の目的

The purpose of this study is to develop computational methods capable of describing the single- and many-particle dynamics of swimmers in complex host solvents using realistic particle models. Our focus is on colloidal particles that use electrophoretic phenomena to generate their propulsion, in general, and ICEP Janus particles in

particular. For this, we aim to describe the propulsion mechanism in detail, which requires that we account for the complex eletro-hydrodynamic/particle coupling responsible for the varied dynamical modes seen in experiments. This computational framework will allow us to understand experiments, as well as propose novel active particle designs for performing specific tasks. In addition, we seek to develop (physics informed) Machine-Learning (ML) methods to accelerate/complement such standard simulation techniques, as well as to help analyze experimental data.

３．研究の方法 (Methods)

The general purpose of this study is to elucidate the complex behaviors of swimming particles, with a focus on ICEP Janus particles. For this, we have employed a Direct Numerical Simulation (DNS) approach, which uses the Smoothed Profile (SP) method to solve for the coupled electro-hydrodynamics and rigid body equations of motion needed to fully describe the ICEP. This particular method can be easily extended to complex host fluids (e.g., phase-separated binary fluids) as well as to account for alternative propulsion mechanisms (e.q., squirmers). Finally, in an effort to accelerate/complement such DNS methods, with the hope of describing the large-scale dynamics of active systems (e.g., learning coarse-grained continuum equations), as well as analyzing experimental data (e.g., reconstructing 3D flow fields), we have developed two physics informed machine learning methods for soft matter flows.

(1) Direct Numerical Simulations of Active Particles

We have extended the Smoothed Profile DNS method to consider the material properties of ICEP Janus particles. This was done by accounting for the (frequency) dependent nonhomogeneous dielectric properties of the system, i.e., allowing for different conductivity/permittivity of the two halves of the Janus colloids, as well as the fluid. In particular, we introduced an additional (Janus) phase-field function, which smoothly distinguishes between the different domains, i.e., the particle head/tail and the fluid. This Janus phase-field was then used to define a complex permittivity field that accounts for the permittivity and the (non-zero) conductivity of the medium. This permittivity field, and the free charge density field (due to the added salt), is used to solve the non-homogenous Poisson equation for the complex electrostatic potential, from which the Maxwell stresses can be calculated. In contrast, the standard formulation of the SP method has so far assumed homogeneous particles that are dielectrically matched to the fluid, considerably simplifying the model. The resulting forces enter into the Navier-Stokes equation for the fluid, as well as the Advection-Diffusion equation for the charged solute, which are coupled to the Newton-Euler equations for the rigid-particles through an additional constraint force on the fluid. Finally, in order to understand the large-scale collective motion of active particles seen experimentally, we have adopted a simplified model of dielectric spheres (i.e., Quincke rollers), in which the electro-hydrodynamic coupling is included through effective interactions. Thus, the rollers are represented as spherical particles with an active Quincke torque (perpendicular to the applied field), with additional effective particle-particle interactions to model the dipole-dipole and electro-osmotic forces.

(2) Machine-Learning flows

Using a Bayesian probabilistic framework based on Gaussian Processes (GP), which provide a probability distribution over functions, we have developed two ML methods applicable to Soft Matter systems. The first method, GP-MSS (Multi-Scale Simulations), allows one to learn the constitutive relation for the stress of Soft Matter flows, which typically possess a hierarchy of time- and length-scales. The relations, learned from microscopic training data, can then be used to perform large-scale flow simulations that are orders of magnitude faster than full MSS. For simplicity, we have developed and tested the method on a well-known example of Soft Matter that exhibits a non-linear rheological response: well-entangled polymer melts. We extended our ML method (Phys. Rev. Res. **02**, 033107, 2020) to infer the (non-linear) constitutive relations of the Doi-Takimoto entanglement model. We only assumed that the stress response (i.e., the time-derivative of the stress) is a function of the local stress and strain, we do not specify its functional form. The second ML method, GPStokes, uses a physics-informed GP regression to infer the solution to arbitrary Stokes flow problems. Crucially, this method ensures that the physics is exactly satisfied. This is done by encoding the Stokes and continuity equations into the GP kernels specifying the correlations among the different fields (e.g., velocity, pressure). The flow inference is performed by

conditioning on all known data. Given that Stokes (low-Reynolds number) flows are characteristic of biological swimmers, as well as high-molecular weight polymer fluids, we expect this method to be applicable to a wide-variety of forward/inverse Soft Matter flow problems.

## 4．研究成果 (Results)

### (1) Direct Numerical Simulations of Active Particles

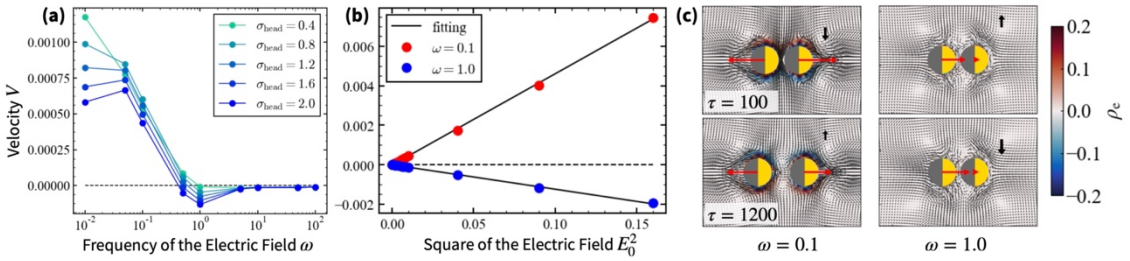


Fig. 1 DNS results for metallo-dielectric Janus particles under AC fields. (a) Propulsion velocity as a function of frequency, for various metal conductivities. (b) Propulsion velocities as a function of the square electric field amplitude, for low and high frequencies, corresponding to forward and reverse motions. (c) A pair of particles for low and high frequencies at two times $\tau$ (colormap shows the solute charge density, vectors the fluid velocity).

We performed DNS simulations of metallo-dielectric Janus particles dispersed in electrolyte solutions under AC/DC fields, in order to study the single-particle dynamics, in particular the velocity reversal observed at high frequencies, as well as the particle-particle interactions. For simplicity, we have considered constant permittivity/conductivity of the head and tail of the Janus particles, representing the metal and dielectric hemispheres, respectively. Under DC fields (3D), we are able to reproduce the non-monotonic velocity dependence on the Debye-length and the permittivity ratio, as predicted by ICEP theory. Under AC fields (2D) we have also reproduced the single particle behaviour observed experimentally. The particle will align itself to move perpendicular to the applied electric field (i.e., metal-dielectric interface parallel to the field). We also observe the velocity reversal as the frequency $\omega$ is increased, which standard ICEP theory cannot predict. In particular, and in contrast to previous proposals, this velocity reversal is observed in bulk, without the need to introduce a conductive wall. Simulations for different conductivities $\sigma$ of the metal half showed that the magnitude of the (reversed) velocity increases with increasing conductivity. For both forward/reverse motion the self-propulsion speed ($V$) depends on the squared amplitude of the field ($E_0^2$), as seen in experiments (Fig.1). Inspection of the flow, charge density, and Maxwell stress/force fields reveals a strong difference between low and high frequencies. The main factor being the charge distribution at the particle surface, which depends on the induced polarization charges and the diffusion time-scale for the counter-ions (i.e., whether or not they are able to respond to the changes in the AC electric field). In particular, when the velocity reversal occurs, a large asymmetry is observed, with strong electric field gradients near the metal/dielectric interface. Simulations of two particles arranged in a head-to-tail configuration reveal that at low frequencies, when counter-ions are able to respond to the field, they accumulate at the particle surface and screen the induced polarization charge, resulting in strong electro-hydrodynamic flows that repel the particles. In contrast, at high frequencies, the charge screening and flow fields are significantly reduced, allowing the particles to move together. This is reminiscent of the chain motion observed experimentally.

We have also performed DNS to study the collective motion of dielectric spheres under DC fields near a wall (i.e., Quincke rollers). Here effective particle-particle interactions are used to account for the electro-hydrodynamic coupling (i.e., the dielectric response and solute charge are not explicitly modelled). The phase-diagram, as a function of particle area fraction $\phi$ and electric field strength $E_0$, reveals a wide variety of collective modes (Fig. 2), e.g., disordered gas, polar liquid, chains, rotating clusters, disordered/polar clusters, and vortex states, most of which have already been observed experimentally. These phases are determined from the interplay between near/far-field hydrodynamics, electrostatic interactions, and their couplings. At low field strengths the particles exhibit weak Quincke rotation, resulting in weak

near-field hydrodynamic interactions, which are dominated by the dipole-dipole interactions. In contrast, at high electric field strengths (and volume fractions) the near-field hydrodynamic interactions dominate and disrupt the alignment.

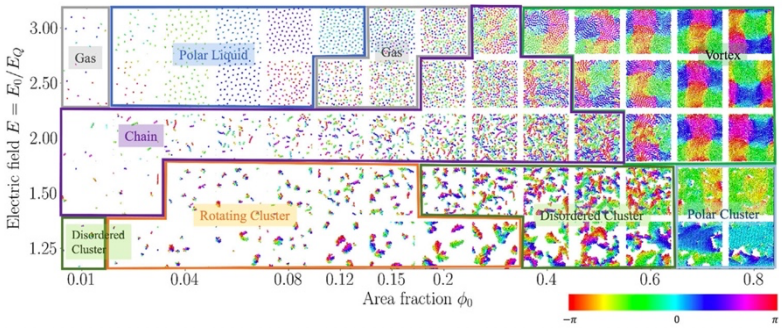


Fig. 2 Phase-diagram for Quincke roller systems, as a function of the scaled Electric field strength and the particle volume fraction. (Imamura et al., Adv. Theory Simul. **6**, 2200683, 2023).

(2) Machine-Learning flows

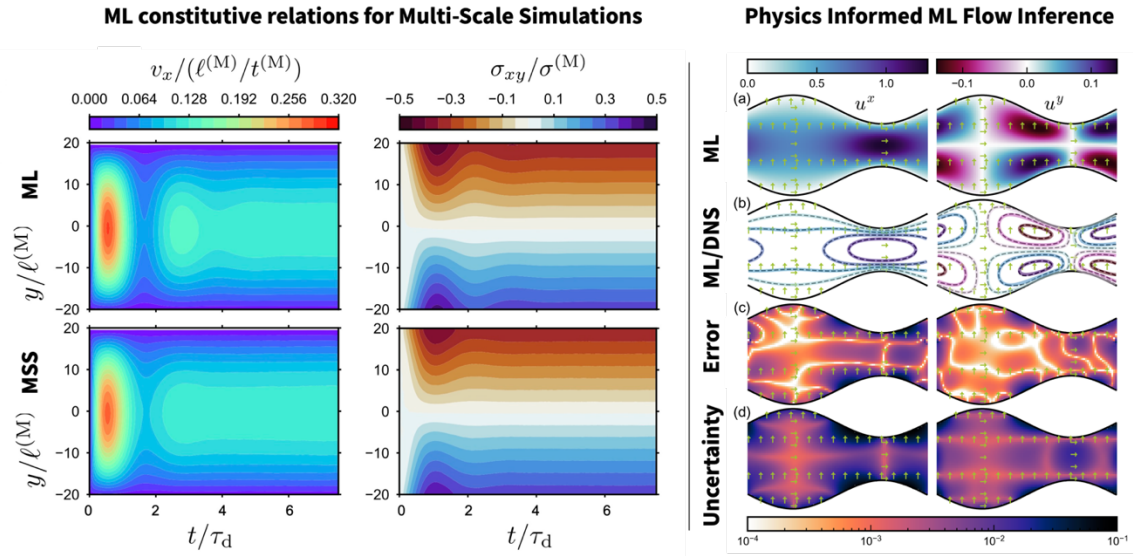


Fig. 3 ML applications for Soft Matter flows. (left) Pressure-driven flow predictions between flat parallel plates, comparing ML and Multi-Scale Simulations. Results show velocity and shear stress as a function of time (adapted from Miyamoto et al., Phys. Fluids, *in press*, 2023). (right) Flow inference using 1D components of the velocity along 1D domains (horizontal/vertical arrows show location of training points for x/y components of the velocity). From top to bottom, ML velocities, ML and DNS velocity contours, ML absolute error, and ML prediction uncertainty.

Our original method for learning constitutive relations was tested on an idealized model of non-entangled polymer melts, i.e., non-interacting Hookean dumbbells that have a linear constitutive relation. Thus, it was unknown whether the method could be applied to more general non-linear systems. We have now extended and validated the method, learning the constitutive relation for a well-entangled polymer melt, as given by the Doi-Takimoto (DT) model. The GP constitutive relations are learned from microscopic training data generated from DT simulations under steady and oscillatory shear-flow. These learned relations are used to perform macroscopic simulations for 2D pressure gap driven flows. To validate our learned constitutive relations, we compare against full multi-scale simulations, which directly embed microscopic DT simulators into the fluid, using $10^4$ polymer chains per SPH fluid particle (see Fig. 3). We obtain excellent agreement between the ML and MSS, with a relative error in the stress predictions of maximum 10%, and the ML simulations are an order of magnitude more efficient (in both compute time and memory). Finally, we have developed a probabilistic Stokes flow framework that is capable of inferring/reconstructing velocity and/or pressure fields from sparse and noisy training data. To test the method, we have considered the pressure driven flow through a sinusoidal channel in 2D. We infer the flows given (i) the full set of boundary conditions (no-slip at the walls and constant pressure gradient), (ii) randomly sampled velocity values (without the boundary conditions), and (iii) 1D components of the velocity along 1D domains (to mimic particle-image velocimetry measurements). In all cases, we obtained excellent agreement with the reference solution obtained from direct numerical simulations (see Fig. 3).

５．主な発表論文等

〔雑誌論文〕　計11件（うち査読付論文　9件／うち国際共著　5件／うちオープンアクセス　3件）

| | |
|---|---|
| １．著者名<br>Miyamoto Souta、Molina John J.、Taniguchi Takashi | ４．巻<br>－ |
| ２．論文標題<br>Machine-learned constitutive relations for multi-scale simulations of well-entangled polymer melts | ５．発行年<br>2023年 |
| ３．雑誌名<br>Physics of Fluids | ６．最初と最後の頁<br>－ |
| 掲載論文のDOI（デジタルオブジェクト識別子）<br>なし | 査読の有無<br>有 |
| オープンアクセス<br>オープンアクセスではない、又はオープンアクセスが困難 | 国際共著<br>－ |

| | |
|---|---|
| １．著者名<br>Feng Chao、Molina John J.、Yamamoto Ryoichi | ４．巻<br>－ |
| ２．論文標題<br>Dynamics of  a model microswimmer in the vicinity of a droplet | ５．発行年<br>2023年 |
| ３．雑誌名<br>Journal of the Physical Society of Japan | ６．最初と最後の頁<br>－ |
| 掲載論文のDOI（デジタルオブジェクト識別子）<br>なし | 査読の有無<br>有 |
| オープンアクセス<br>オープンアクセスではない、又はオープンアクセスが困難 | 国際共著<br>－ |

| | |
|---|---|
| １．著者名<br>Sankaewtong Krongtum、Molina John J.、Turner Matthew S.、Yamamoto Ryoichi | ４．巻<br>107 |
| ２．論文標題<br>Learning to swim efficiently in a nonuniform flow field | ５．発行年<br>2023年 |
| ３．雑誌名<br>Physical Review E | ６．最初と最後の頁<br>065102 (11 pp) |
| 掲載論文のDOI（デジタルオブジェクト識別子）<br>10.1103/PhysRevE.107.065102 | 査読の有無<br>有 |
| オープンアクセス<br>オープンアクセスではない、又はオープンアクセスが困難 | 国際共著<br>該当する |

| | |
|---|---|
| １．著者名<br>Feng Chao、Molina John J.、Turner Matthew S.、Yamamoto Ryoichi | ４．巻<br>35 |
| ２．論文標題<br>Dynamics of microswimmers near a liquid-liquid interface with viscosity difference | ５．発行年<br>2023年 |
| ３．雑誌名<br>Physics of Fluids | ６．最初と最後の頁<br>051903 (14 pp) |
| 掲載論文のDOI（デジタルオブジェクト識別子）<br>10.1063/5.0148008 | 査読の有無<br>有 |
| オープンアクセス<br>オープンアクセスではない、又はオープンアクセスが困難 | 国際共著<br>該当する |

| | |
|---|---|
| １．著者名<br>Feng Chao、Molina John J.、Turner Matthew S.、Yamamoto Ryoichi | ４．巻<br>4 |
| ２．論文標題<br>Dynamics of microswimmers near a soft penetrable interface | ５．発行年<br>2022年 |
| ３．雑誌名<br>Physical Review Research | ６．最初と最後の頁<br>043202 (9 pp) |
| 掲載論文のDOI（デジタルオブジェクト識別子）<br>10.1103/PhysRevResearch.4.043202 | 査読の有無<br>有 |
| オープンアクセス<br>オープンアクセスとしている（また、その予定である） | 国際共著<br>該当する |

| | |
|---|---|
| １．著者名<br>Imamura Shun、Sawaki Kohei、Molina John J.、Turner Matthew S.、Yamamoto Ryoichi | ４．巻<br>6 |
| ２．論文標題<br>Collective Motion of Quincke Rollers with Fully Resolved Hydrodynamics | ５．発行年<br>2023年 |
| ３．雑誌名<br>Advanced Theory and Simulations | ６．最初と最後の頁<br>2200683 (10 pp) |
| 掲載論文のDOI（デジタルオブジェクト識別子）<br>10.1002/adts.202200683 | 査読の有無<br>有 |
| オープンアクセス<br>オープンアクセスではない、又はオープンアクセスが困難 | 国際共著<br>該当する |

| | |
|---|---|
| １．著者名<br>Miyamoto Souta、Molina John J.、Taniguchi Takashi | ４．巻<br>87 |
| ２．論文標題<br>からみ合い高分子溶融体の流動解析手法の進展 ： マルチスケールシミュレーション法と機械学習の融合 | ５．発行年<br>2023年 |
| ３．雑誌名<br>化学工学会誌 | ６．最初と最後の頁<br>111～113 |
| 掲載論文のDOI（デジタルオブジェクト識別子）<br>なし | 査読の有無<br>無 |
| オープンアクセス<br>オープンアクセスではない、又はオープンアクセスが困難 | 国際共著<br>－ |

| | |
|---|---|
| １．著者名<br>Taniguchi Takashi、Molina John J. | ４．巻<br>35 |
| ２．論文標題<br>Machine Learning for the Flow Prediction of Fluids with Memory Effects on the Stress | ５．発行年<br>2021年 |
| ３．雑誌名<br>Japanese Journal of Multiphase Flow | ６．最初と最後の頁<br>426～436 |
| 掲載論文のDOI（デジタルオブジェクト識別子）<br>10.3811/jjmf.2021.t008 | 査読の有無<br>無 |
| オープンアクセス<br>オープンアクセスとしている（また、その予定である） | 国際共著<br>－ |

| | |
|---|---|
| 1．著者名<br>Yamamoto Ryoichi、Molina John J.、Nakayama Yasuya | 4．巻<br>17 |
| 2．論文標題<br>Smoothed profile method for direct numerical simulations of hydrodynamically interacting particles | 5．発行年<br>2021年 |
| 3．雑誌名<br>Soft Matter | 6．最初と最後の頁<br>4226～4253 |
| 掲載論文のDOI（デジタルオブジェクト識別子）<br>10.1039/D0SM02210A | 査読の有無<br>有 |
| オープンアクセス<br>オープンアクセスとしている（また、その予定である） | 国際共著<br>－ |

| | |
|---|---|
| 1．著者名<br>Fadda Federico、Molina John Jairo、Yamamoto Ryoichi | 4．巻<br>101 |
| 2．論文標題<br>Dynamics of a chiral swimmer sedimenting on a flat plate | 5．発行年<br>2020年 |
| 3．雑誌名<br>Physical Review E | 6．最初と最後の頁<br>52608 (11 pp) |
| 掲載論文のDOI（デジタルオブジェクト識別子）<br>10.1103/PhysRevE.101.052608 | 査読の有無<br>有 |
| オープンアクセス<br>オープンアクセスではない、又はオープンアクセスが困難 | 国際共著<br>－ |

〔学会発表〕　計31件（うち招待講演　3件／うち国際学会　19件）

| |
|---|
| 1．発表者名<br>Souta Miyamoto (*), John J. Molina, Takashi Taniguchi |
| 2．発表標題<br>Applications of machine-learned constitutive relations to simulate well-entangled polymer melt flows |
| 3．学会等名<br>PPS-37 : The 37th International Conference of the Polymer Processing Society（国際学会） |
| 4．発表年<br>2022年 |

| |
|---|
| 1．発表者名<br>Kenta Ogawa, John J. Molina (*), Takashi Taniguchi |
| 2．発表標題<br>Flow Problems as Inference Problems |
| 3．学会等名<br>PPS-37 : The 37th International Conference of the Polymer Processing Society（国際学会） |
| 4．発表年<br>2022年 |

１．発表者名
Chao Feng (*), John J. Molina, Matthew S. Turner, Ryoichi Yamamoto

２．発表標題
Dynamics of micro-swimmers near deformable and penetrable interfaces

３．学会等名
APPC15 : The 15th Asia Pacific Physics Conference（国際学会）

４．発表年
2022年

１．発表者名
Krongtum Sankawtong (*), John J. Molina, Matthew S. Turner, Ryoichi Yamamoto

２．発表標題
Learning to swim efficiently in a nonuniform flow field

３．学会等名
ISMC 2022 : The International Soft Matter Conference（国際学会）

４．発表年
2022年

１．発表者名
Souta Miyamoto (*), John J. Molina, Takashi Taniguchi

２．発表標題
Machine-learned constitutive relations for simulating well-entangled polymer melts for their history-dependent flows

３．学会等名
The Society of Rheology 93rd Annual Meeting（国際学会）

４．発表年
2022年

１．発表者名
John J. Molina (*), Kenta Ogawa, Souta Miyamoto, Takashi Taniguchi

２．発表標題
Machine Learning Physics for Flowing Soft Matter

３．学会等名
25th Anniversary Symposium of German-Japanese Joint Research Project on Nonequilibrium Statistical PHysics Perspective for Future Collaboration（招待講演）（国際学会）

４．発表年
2022年

１．発表者名
John J. Molina (*), Takuya Eriguchi, Ryoichi Yamamoto

２．発表標題
Direct Numerical Simulation of Metallodielectric Janus Particles

３．学会等名
APS March Meeting 2023（国際学会）

４．発表年
2023年

１．発表者名
John J. Molina (*), Simon K. Schnyder, Matthew S. Turner, Ryoichi Yamamoto

２．発表標題
Physics Informed Machine Learning for (Inverse) Optimal Control

３．学会等名
第10回ソフトマター研究会

４．発表年
2022年

１．発表者名
Chao Feng (*), John J. Molina, Matthew S. Turner, Ryoichi Yamamoto

２．発表標題
Direct numerical simulations of a model microswimmer near a liquid-liquid interface

３．学会等名
Active Matter Workshop 2023

４．発表年
2023年

１．発表者名
John J. Molina (*), Souta Miyamoto, Takashi Taniguchi

２．発表標題
Learning the constitutive relation of polymer melt flows

３．学会等名
The 2021 International Chemical Congress of Pacific Basin Societies (Pacifichem 2021)（国際学会）

４．発表年
2021年

１．発表者名
Shun Imamura (*), Kohei Sawaki, John J. Molina, Ryoichi Yamamoto

２．発表標題
Collective Dynamics of Quincke Rollers with Fully Resolved Hydrodynamics

３．学会等名
American Physical Society (APS) March Meeting 2022（国際学会）

４．発表年
2022年

１．発表者名
Souta Miyamoto (*), John J. Molina, Takashi Taniguchi

２．発表標題
Application of Machine-learned constitutive relations for well-entangled polymer melt flows

３．学会等名
American Physical Society (APS) March Meeting 2022（国際学会）

４．発表年
2022年

１．発表者名
John J. Molina (*), Simon K. Schnyder, Matthew S. Turner, Ryoichi Yamamoto

２．発表標題
Nash Neural Networks

３．学会等名
American Physical Society (APS) March Meeting 2022（国際学会）

４．発表年
2022年

１．発表者名
Souta Miyamoto (*), John J. Molina, Takashi Taniguchi

２．発表標題
学習された構成関係を用いた高分子液体の流動シミュレーション

３．学会等名
化学工学会 第52回秋季大会(2021)

４．発表年
2021年

１．発表者名
Souta Miyamoto (*), John J. Molina, Takashi Taniguchi

２．発表標題
Well-entangled polymer melt flow simulations using a Machine-Learned constitutive relation

３．学会等名
第69回レオロジー討論会

４．発表年
2021年

１．発表者名
John J. Molina (*), Takashi Taniguchi

２．発表標題
A Machine Learning Approach to Flow Problems

３．学会等名
第69回レオロジー討論会

４．発表年
2021年

１．発表者名
Souta Miyamoto (*), John J. Molina, Takashi Taniguchi

２．発表標題
機械学習モデルを構成関係に代用した高分子溶融体の流動シミュレーション

３．学会等名
プラスチック成形加工学会第29回秋季大会

４．発表年
2021年

１．発表者名
John J. Molina (*), Takashi Taniguchi

２．発表標題
Gaussian Processes for Machine Learning of Fluid Flows

３．学会等名
ソフトバイオ研究会2021（招待講演）

４．発表年
2021年

１．発表者名
John J. Molina(*)

２．発表標題
Novel Soft Matter Physics through Computational and Information Science (oral)

３．学会等名
The Physical Society of Japan 2021 Annual Meeting (online)（招待講演）

４．発表年
2021年

１．発表者名
Takuya Eriguchi(*)、John J. Molina

２．発表標題
Direct Numerical Simulation of Induced Charge Electrophoresis of Janus Particles

３．学会等名
68th Annual Meeting of the Society of Rheology of Japan (online)

４．発表年
2020年

１．発表者名
John J. Molina(*)、Naoki Seryo、Takeshi Sato, Takashi Taniguchi

２．発表標題
Learning the Constitutive Relation of Polymer Flows with Memory: from Micro-Scale Dynamics to Macro-Scale Flow

３．学会等名
SIAM Conference on Computational Science and Engineering (online)（国際学会）

４．発表年
2021年

１．発表者名
Federico Fadda(*)、John J. Molina、Ryoichi Yamamoto

２．発表標題
Sedimenting chiral swimmers

３．学会等名
Americal Physical Society (APS) March Meeting 2021 (online)（国際学会）

４．発表年
2021年

〔図書〕　計0件

〔産業財産権〕

〔その他〕

―

6．研究組織

| | 氏名<br>（ローマ字氏名）<br>（研究者番号） | 所属研究機関・部局・職<br>（機関番号） | 備考 |
|---|---|---|---|
| 研究協力者 | 山本　里一<br>(Yamamoto Ryoichi)<br>(10263401) | | |
| 研究協力者 | 谷口　貴志<br>(Taniguchi Takashi)<br>(60293669) | | |

7．科研費を使用して開催した国際研究集会

〔国際研究集会〕　計0件

8．本研究に関連して実施した国際共同研究の実施状況

| 共同研究相手国 | 相手方研究機関 |
|---|---|