1-1-2020

Directed Assembly of Binary Magnetic Particles

Isaac Torres-Diaz
University of Alabama in Huntsville

Directed Assembly of Binary Magnetic Particles

Isaac Torres Díaz

Assistant Professor

Department of Chemical and Materials Engineering

301 Sparkman Drive.

Engineering Building 117B

256-824-3596, isaac.torres.diaz@uah.edu

RCEU20-CHE-ITD-02

Project Description

Anisotropic colloidal particles are of great interest for the bottom-up assembly of materials. They are used as building blocks to assemble materials with non-conventional properties not available in nature. Uniform anisotropic colloids have directional and tunable interactions compared with uniform spherical particles. Currently, there is available a large variety of anisotropic colloids for self–assembly and directed–assembly, which are classified by the shape anisotropy (e.g., superellipsoids), surface anisotropy (e.g., Janus particles), branchiness (e.g., dendritic particles), and the internal configuration (e.g., ordered lamellar colloids). The variety of anisotropic colloids can promote a multiverse of synthetic structures, where the equilibrium configuration is determined by entropic effects and by the directional interactions between the anisotropic particles, such as the dipolar interactions between particles under the influence of a magnetic field. Modeling a large number of magnetic anisotropic particles, including the dipolar interactions, is necessary to predict and engineer new synthetic materials.

On this project, we will investigate and predict the equilibrium configuration of magnetic anisotropic colloidal particles confined in a two-dimensional space using Monte Carlo simulation. The project will focus on the analysis of binary magnetic particles, where we will study the influence of aspect ratio between the anisotropic colloids on the equilibrium configuration. As a result, we will develop an algorithm capable of describing the most probable equilibrium configuration of binary particles under the influence of a uniform magnetic field, which will be used in the assembly of novel materials.

Previously, we have analytically and experimentally quantified the interaction energy of the induced dipole with the electric field. Additionally, we simulated uniform anisotropic particles under the influence of alternating non-uniform electric fields, where we predict four different equilibrium configurations of the tunable structure. Additionally, we used order parameters and pair correlation functions to characterize the phases of hard superellipsoids. In the proposed work, we will use Monte Carlo simulation to model the assembly of binary magnetic colloids with shape anisotropy, which interact under the influence of a magnetic field on a two-dimensional confinement.

Student Duties, Contributions, and Outcomes

Specific Duties: The student must perform the simulations, plot the results, analyze the data, and write reports on a regular basis during the summer. For that purpose, the student will have a computer station where to perform the simulations and a hard drive to store/backup the data. Additionally, the student must review the current literature in the field regularly under the guidance of the Professor and the graduate students. Furthermore, the student will present his/her results three times during the summer in group meetings. It is expected to submit two reports during his/her stay during the summer, a midterm report, and a final report.

Tangible Contributions: It is expected that the student publishes his/her final results in Perpetua, and present his/her results in the poster session during the fall at UAH. The extended version of the final report, in collaboration with the graduate student and under the supervision of the Faculty, will be published in a peer-review Journal.

Specific Outcomes: The student will learn how to quantify the interaction energy landscape between objects as a function of position and orientation. The student will learn computational tools (e.g., Unix/Linux, Matlab, Fortran, and Wolfram Mathematica) relevant for different computational research work. Additionally, the student will learn important concepts about translation and rotation of small colloidal particles and how to model the relative interaction between them. The student will learn how to analyze, plot, and calculate the average components of a multi-dimensional energy landscape. The student will work in a research environment, participating in research discussions, and collaborating with graduate students for writing a peer review article. The interaction with other graduate students will be a valuable experience for future undergrad or graduate research experiences.

Student Selection Criteria

This project is open to highly motivated students at all academic ranks from the college of Sciences and the College of Engineering.

Faculty/Research Staff Mentorship

The Professor will train the student daily during the first two weeks (or longer) of the project to ensure the student learns and handles the computational tools required to accomplish the project. After that, the student will meet the Professor every other day to present one or two slides about his/her research results achieved during the previous days. The Professor will advise the next steps in the research to be accomplished before the next meeting, i.e., the Professor will ensure the student success in the undergraduate summer project with permanent guidance as to any other graduate student. Additionally, the daily informal conversations with the Professor every time that he steps in the laboratory or the undergraduate student requires it to overcome any research problem. Furthermore, the student will interact with a Ph.D. student and a Master's student while the research project is completed. Fully trained graduate students will be the first contact persons in the computational laboratory to answer his/her questions related to the research topic.