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Interaction of Internally-structured Anisotropic Particles with Substrates

Isaac Torres-Diaz
University of Alabama in Huntsville

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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

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Project Description

Currently, there is an increasing interest in using colloidal particles with shape anisotropy as nanocarriers to deliver encapsulated drugs at specific locations in the organism. Anisotropic particle needs to be compatible with its local environment and being selective to the drug and the targeted cell. In particular, anisotropic colloids are of great importance because of their directional interactions compared with uniform spherical particles. There is a large variety of anisotropic colloids, which can be classified by the shape (e.g., ellipsoids and superellipsoids), the surface anisotropy (e.g., Janus and patchy particles), branchiness (e.g., hexapods and dendritic particles), and internally structured configuration (e.g., ordered lamellar colloids). The internally structured colloids provide multiple surface chemistry sites that allow a multifunctional interaction, such as with drugs and cell membranes. Quantifying the interaction of internally-structured colloids with substrates is a crucial factor in predicting, maximizing, and engineering nanocarriers with specificity for different cell environments.

On this project, we will investigate the interactions of internally-structured anisotropic particles with a planar substrate, which will serve as a simplified model for a multifunctional nanocarrier close to a cell membrane. We will quantify the DLVO (Electrostatic and van der Waals) interactions for colloid at different positions and orientations, and as a function of the particle shape, aspect ratio, and structured configuration. As a result, we will develop an algorithm capable of describing the most probable equilibrium configuration of small-particles near a flat surface.

Previously, we have quantified the DLVO interactions for uniform superellipsoids, toroid, and buckle colloidal particles using Derjaguin approximation. In the proposed work, we will use the surface-element-integration method to improve the quantification of the interactions of internally structured colloids with a planar wall.

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 he/she will 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 Faculty and the graduate students. Furthermore, the student will present his/her results three times during the summer in group meetings. It is expected that the student submits 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 microparticles or nanoparticles as a function of position and orientation. The student will learn computational tools (e.g., Matlab, Fortran, Wolfram Mathematica, and specialized rendering software) 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 them close to a planar wall. 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 P.I. 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 P.I. 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 P.I. 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.