A STUDY ON THE DYNAMICS AND SELF-ASSEMBLY OF ANISOTROPIC PARTICLES

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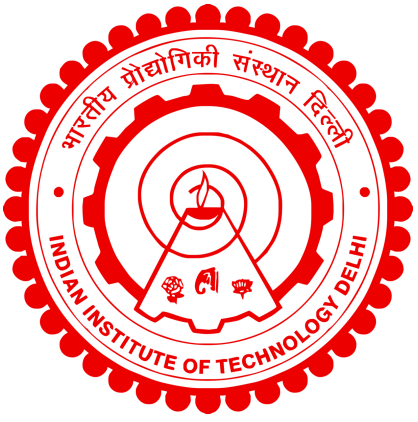

DEPARTMENT OF PHYSICS

INDIAN INSTITUTE OF TECHNOLOGY DELHI

FEBRUARY 2024

A STUDY ON THE DYNAMICS AND SELF-ASSEMBLY OF ANISOTROPIC PARTICLES

by

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Department of Physics

Submitted

in fulfillment of the requirements of the degree of

Doctor of Philosophy

to the

INDIAN INSTITUTE OF TECHNOLOGY DELHI

FEBRUARY 2024

Dedicated to my uncle and Gurudev Shree Harihar

Certificate

This is to certify that the thesis entitled **"A STUDY ON THE DYNAMICS AND SELF-ASSEMBLY OF ANISOTROPIC PARTICLES"**, submitted by **VIKKI ANAND VARMA, Entry No. 2018PHZ8362** to the Indian Institute of Technology Delhi, for the award of the degree of **Doctor of Philosophy** in **PHYSICS**, is a record of the original, bonafide research work carried out by him under our supervision and guidance. The thesis has reached the standards fulfilling the requirements of the regulations related to the award of the degree.

The results contained in this thesis have not been submitted in part or in full to any other University or Institute for the award of any degree or diploma to the best of our knowledge.

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Acknowledgements

I want to thank my supervisor **Prof. Sujin B. Babu** for his guidance and support. I would also like to thank my mentors **Dr. Isha Malhotra**, and **Dr. Mohd Yasir Khan**. I am thankful to my beloved seniors **Dr. Shahrukh Salim**, **Dr. Vikas Mishra** and **Dr. Harsh Gupta** for consistently supporting me and teaching me philosophy and physics during our badminton games. I am thankful to the members of my SRC committee **Prof. Pradipta Ghosh**, **Prof. Varsha Banerjee**, and **Prof. Vikram Singh**. I would also like to acknowledge my seniors, Yatin Pitkar and Sooryansh Asthana for consistently supporting and caring me. And Simmie, for helping me in and out of the lab. I am thankful to my juniors for their love and support, especially Kritika, Jaskaran, Mintu, and Roshan. I would also like to thank my room partners and friends, Dr. Vimarsh Awasthi, Divyanshu Vikram Singh, Ajay Kumar, Fauzia Khan and Shubham Tiwari. In the end, I would like to thank my robotic friend Om Shankar.

Vikki Anand Varma

Abstract

The thesis primarily focuses on the different aspects of dynamical and structural properties arising mainly due to the shape-anisotropy of the particles within a colloidal system. We studied the diffusivity of the particles in a one-component system. The friction effect dominates the diffusivity of spheroids at lower volume fractions. While at higher volume fractions, it depends upon structural properties like phases and random packing. In the two-component system, the diffusivity of the spheroids has been observed to increase in the presence of spheres as the secondary component. The nematic phases have been observed destroying in the presence of spheres, leading to a fraction of spheres vs volume-fraction phase diagram. Later in the work, we studied the self-assembly of spheroids with directional and limited bonding using patches. We found shape anisotropy working along with the directional bonding, forming a phase-rich system. Within a particular range of anisotropy, the system could lead to the formation of complex structures like a free-standing monolayer. In the later part, we used annular patches to study the cause of disordering arising in constructing a spherical shell. We found that both icosahedral symmetry and disordered shells show the same potential energy. Therefore, due to the lack of the deriving force in an axially symmetric potential, we found the absence of icosahedral symmetry despite the shell's spherical shape. Flexibility in structural rearrangement plays an essential role in forming close spherical shells via the self-assembly approach. However, the shells are ideal for drug delivery due to their large enough size and spherical shape to trap the particles inside.

सारांश

यह अनुसंधान कार्य मुख्य रूप से कोलाइडल प्रणाली के भीतर कणों के आकार- अनिसोट्रॉपी के कारण उत्पन्न होने वाले गति शील और संरचनात्मक गुणों के विभिन्न पहलुओं पर केंद्रित है। हमने एक-घटक प्रणाली में कणों की विसरणशीलता का अध्ययन कि या। घर्षण प्रभाव कम मात्रा वाले अंशों पर कण की विसरणशीलता पर दमनात्मक होता है। जबकि उच्च मात्रा वाले अंशों पर, यह चरणों और याद्दच्छिक पैकिंग जैसे संरचनात्मक गुणों पर निर्भर करता है। दो-घटक प्रणाली में, द्वितीयक घटक के रूप में गोले की उपस्थिति में कण की प्रसारशीलता में वृद्धि देखी गई है। नेमैटिक चरणों को गोले की उपस्थिति में नष्ट होते हुए देखा गया है, जिससे कण का एक अंश बनाम आयतन-अंश चरण आरेख बनता है। बाद में काम में, हमने पैच का उपयोग करके दि शात्मक और सीमित बॉन्डिंग के साथ कण के स्व-संयोजन का अध्ययन कि या। हमने पाया कि आकार-अनिसोट्रॉपी दिशात्मक बंधन के साथ मिलकर एक चरण-समृद्ध प्रणाली का निर्माण करती है। आकार- अनिसोट्रॉपी की एक विशेष सीमा के भीतर, सि स्टम एक मुक्त- खड़े मोनोलेयर जैसी जटिल संरचनाओं के निर्माण का कारण बन सकता है। बाद के भाग में, हमने गोलाकार खोल के नि र्माण में उत्पन्न होने वाली गड़बड़ी के कारण का अध्ययन करने के लि ए कुंडलाकार पैच का उपयोग किया। हमने पाया कि इकोसाहेड्रल समरूपता और अव्यवस्थित गोले दोनों समान संभावित ऊर्जा दिखाते हैं। इसलिए, अक्षीय रूप से सममित क्षमता में व्युत्पन्न बल की कमी के कारण, हमने शेल के गोलाकार आकार के बावजूद आइकोसाहेड्रल समरूपता की अनुपस्थिति पाई। संरचनात्मक पुनर्व्यवस्था में लचीलापन स्व-संयोजन दृष्टिकोण के माध्यम से लगभग गोलाकार गोले बनाने में एक आवश्यक भूमि का निभाता है। यद्यपि , गोले अपने बड़े आकार और कणों को अंदर फंसाने के गुण के कारण दवा वितरण के लिए आदर्श होते हैं।

Contents

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Abbreviations

BCD	**B**rownian **C**luster **D**ynamics
DLCA	**D**iffusion **L**imited **C**luster **A**ggregation
EDBD	**E**vent **D**riven **B**rownian **D**ynamics
ECF	**E**llipsoid **C**ontact **F**unction
OBB	**O**bject **B**ounding **B**ox
ER	**E**llipsoid of **R**evolution
MSD	**M**ean **S**quare **D**isplacement
KFP	**K**ern **F**renkel **P**oltential
MD	**M**olecular **D**ynamics
MC	**M**onte **C**arlo
SGMC	**S**emi **G**rand-canonical **M**onte **C**arlo
US	**U**mbrella **S**ampling
HC	**H**ard **C**ore

Symbols

k_B	Boltzman constant
T	temperature
p	pressure
ϕ	volume fraction
N	number of particles
d	diameter of sphere
L	simulation box size
$\hat{n}$	director of spheroids
$D_\circ^T$	Translational diffusivity of a single sphere suspended in colloidal solution
$D_\circ^R$	Rotational diffusivity of a single sphere suspended in colloidal solution
G_θ	Perrin's friction factor for rotational motion
$G_\parallel$	Perrin's friction factor for translational motion along the director
$G_\perp$	Perrin's friction factor for translational motion perpendicular to the director
γ	Friction coefficient
η	Viscosity
s_T	translational step length
s_R	rotational step length
t_{Phy}	physical time
t_{Sim}	simulation time
$t_\circ$	time taken by a single sphere to diffuse through the length of its own diameter
PBC	periodic boundary condition