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Name: **Dr. Partha Sarathi Majee (Principal Investigator)**

Department: **Mathematics**

Project Title: **Numerical Investigations Supplemented with Theoretical Analysis on Diffusiophoresis of Composite Nanoparticles.**

Funding Agency: **ANRF-ARGM (Anusandhan National Research Foundation – Advanced Research Grant – Mathematical)**

Sanction Amount: **3000000 Lakhs**

Fund Utilised.: 0

Tenure: **5 Years**

Abstract:

The present proposal strive to conduct numerical simulations and theoretical analysis on the diffusiophoresis of soft nanoparticles. Diffusiophoresis refers to the migration of charged particles under the influence of an external concentration gradient, which finds extensive applications in manipulation of organic cells, targeted drug delivery, particles separation, DNA translocation, enhanced oi recovery, and water filtration, among others. Soft particles, comprising a rigid core coated with a polyelectrolyte layer, can effectively emulate viruses, bacteria, fabricated nanoparticles, and humic substances, are highly significant in colloid science.

The prime objective is to analyze the diffusiophoresis of soft particles in various electrokinetic environments, such as 1) surface charge mobility dependent hydrophobic inner core, 2) pH dependent particles charge, 3) ion-steric repulsion, and 4) ion partitioning effect. One main focus is to derive closed-form expressions and semi-analytic solutions for the diffusiophoretic mobility. Other objectives include analysing the impact of the high charge-induced nonlinear effects, such as double layer polarization, and counter ion condensation, on the flow. The mathematical model to be employed is based on coupled Brinkman-extended Navier-Stokes, Nernst-Planck, and Poisson equations and will be solved numerically. The successful completion of the project will yield closed-form expression for diffusiophoretic mobility and a thorough understanding of the fow in the mentioned situations.

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