Proposal Review 1 : 2206369

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Agency Name:	National Science Foundation
Agency Tracking Number:	**2206369**
Organization:	
NSF Program:	APPLIED MATHEMATICS
PI/PD:	Quaife, Bryan
Application Title:	Collaborative Research: Mathematical modeling and simulation of self-assembling amphiphilic particles in solvent
Rating:	Multiple Rating: (Very Good/Good)

Review

Summary

In the context of the five review elements, please
evaluate the strengths and weaknesses of the proposal with respect to intellectual merit.

Overview: This project proposes to study/extend a recent framework introduced by two of the three PIs, HAP (hydrophobic attraction potential), to model the self-assembly process of rigid (non-deforming) amphiphilic particles in solvent.

The basic idea is to solve the Stokes flow of a suspension of rigid spherical particles that feature on their surface a prescribed stress vector that arises from the minimization of a free-energy functional for an order parameter u. Different choices for the potential f(u) and boundary condition g in that functional lead to different behaviors.

Specifically, three Aims are proposed:

Aim 1 is concerned with the study of the HAP formulation for various choices of f(u) and g.

Aim 2 is concerned with the development of a numerical scheme to solve the resulting equations for u in Aim 1.

Aim 3 is concerned with the extension of the HAP formulation to Stokes flow in the presence of ions and their transport.

Strengths: The HAP formulation does appear as an interesting approach to account for local features in the self-assembly process of amphiphilic particles while remaining in the continuum and hence numerically efficient.

Weaknesses: The physical problems that will be studied are not specified. For instance, what are the flows that will be considered (i.e., the boundary conditions on the solvent)? How many particles will be considered? What sizes of particles will be considered? Etc. A brief mention of these seems necessary to clarify the fundamental problems that the PIs have in mind and where they stand within the state of the art.

The connection between the inputs entering the proposed HAP formulation and experimental observations is not sufficiently elaborated. It is thus unclear how progress in the modeling and numerical implementation as proposed may advance fundamental knowledge of the actual self-assembly process of amphiphilic particles.

In the context of the five review elements, please
evaluate the strengths and weaknesses of the proposal with respect to broader impacts.

Strengths: The self-assembly of amphiphilic particles in solvent is an ubiquitous phenomenon in biology and soft matter at large. Advances in its quantitative description is hence likely to have an impact in a variety of applications.

The project will meaningfully involve undergraduate students.

Weaknesses: It can be inferred from the budget that two graduate students will also be involved in the project, but this does not appear to be stated in the project description. The specific contributions by each of the three PIs and their integration lacks some clarity.

Please evaluate the strengths and
weaknesses of the proposal with respect to any additional solicitation-specific review criteria, if
applicable

Summary Statement

The proposed HAP formulation to study the self-assembly process of amphiphilic particles appears to be interesting. Its connection with experimental observations, however, is not sufficiently detailed. Similarly, the specific contributions by each of the three PIs and their integration is not sufficiently detailed.

This proposal ranks in the top third of the proposals that I have reviewed.