Agency Name:
National Science Foundation
Agency Tracking Number:
2009898

Panel Summary

Panel Summary

BRIEF SUMMARY OF PROJECT

The project is aimed at developing mathematical models for the collective dynamics of amphiphilic particles and their self-assembly.

INTELLECTUAL MERIT

Strengths: The proposal is from a team of collaborators coming from mathematics and physics who are well qualified.

The proposal is well written and quite clear. The panel noted that the development of 3D models describing colloidal system could be transformative and has a potential to model complex systems. The numerical simulations use new approaches with a potential to compute with less cost than molecular dynamics. The simulated preliminary results show its promise. The panel agreed proposed projects address questions that are out of reach today in the computational material science area.

Weaknesses: The panel noted that out of three one PIs, one is an expert in scientific computing and the other two in mathematics and physics.

However, it is not clear what novel mathematics is involved as the model is already established. The panel also thought the proposal lacked the necessary mathematical component which could give fundamental insight for the success of the proposed research.

BROADER IMPACTS

The proposal will have a good educational impact via student training.

Results of Prior NSF Support:

Results from prior support are strong.

Postdoctoral Mentoring Plan:

RECOMMENDATION

This was a good proposal but the panel thought the lack of strong mathe-maticall component made it less competitive compared to other proposals.

The panel placed this proposal in the category: Not Competitive.

This summary was read by/to the panelists and they concurred that the summary accurately reflects the panel discussion.
PANEL RECOMMENDATION: Not Competitive

Review #3

Agency Name:
National Science Foundation
Agency Tracking Number:
2009898
Organization:

NSF Program:
APPLIED MATHEMATICS
PI/PD:
Ryham, Rolf
Application Title:
Collaborative Research: Mathematical modeling and coarse-grained simu-lations of self-assembly of amphiphilic Janus particles in a solvent
Rating:
Very 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.

The project addresses modeling (especially numerical modeling) of systems with many interacting amphiphilic particles. Due to non-additivity and hydrophobic attraction, colloidal systems self-assemble into bilayer morphologies. Properties of these ensembles are analyzed. The simulation is performed by a variant of boundary integral equation quadratures in three dimensions; it accounts for collisions. The results allow the modeling of complex systems that are out of reach today. The plan is well-organized, the team of collaborators is well qualified.

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

The developed methods will be used for modeling a range of practically important systems, from metamaterials to bio-systems. The collaboration is beneficial for graduate students involved in the project. Pis plan to mentor undergraduate students.

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

Summary Statement

This proposal addresses novel and important problems. I recommend funding it.

Review #2

Agency Name:
National Science Foundation
Agency Tracking Number:
2009898

Organization:

NSF Program:
APPLIED MATHEMATICS
PI/PD:
Ryham, Rolf
Application Title:
Collaborative Research: Mathematical modeling and coarse-grained simulations of self-assembly of amphiphilic Janus particles in a 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.

This is a collaborative proposal from two PIs (mathematician and physicist) and one co-PI (numerical scientist) presenting mathematical modeling of biological membranes. The PIs developed a mathematical model called the hydrophobic attraction potential (HAP) recently. This model may reach many interesting physical phenomena with less computational cost than molecular dynamics, but possessing more general features, granularity of lipid molecules, that continuum theory misses. The PIs propose to develop efficient higher order numerical methods for HAP and compare results with pre-existing theory and experimental measurements. The PIs expect to measure elastic constants that are consistent with experiment with HAP theory and apply for the fabrication of functional materials.

The project is about developing new efficient numerical algorithm and performing the simulations to solve some disparities from experiments and theories. Also, the PIs show preliminary results on membranes and 3d objects from simulations.

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

PI Royham plans to advise undergraduate students at Fordham university in this interdisciplinary subject and the PI Young and co-PI Jiang continue to advise a female graduate student at NJIT.

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

Summary Statement

This is a good research proposal enhancing the mathematical modeling of biological membranes and more materials and develop an efficient numerical method. I rank it within the middle third of those reviewed.

Review #1

Agency Name:
National Science Foundation
Agency Tracking Number:
2009898
Organization:

NSF Program:
APPLIED MATHEMATICS
PI/PD:
Ryham, Rolf
Application Title:
Collaborative Research: Mathematical modeling and coarse-grained simulations of self-assembly of amphiphilic Janus particles in a 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.

This project aims to advance the mathematical modeling of the collective dynamics of amphiphilic particles, with main focuses on their self-assembly, fusion and fission of amphiphilic bilayer membranes, and optimal shape designs for specific functions. The main ingredients of the physical model

includes nonlocal interactions between Janus particles mediated by solvent that mimics a kind of “screen” potential and the classical hydrodynamics. It turns out that this “minimal” model gives rise to rich phenomena for Janus aggregates as shown by the PIs. The technical research tasks include (1) Elastic properties of amphiphile ensembles, (2) Efficient high-order numerical algorithm for large-scale simulation of the HAP model, and (3) achieving design and self-assembly of functional materials by Janus particles.

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

The broader impact of the proposal looks strong. The scientific outcome may be transformative in terms of collective dynamics of Janus particles with nonlocal interactions. Outreach efforts include supporting women students and other underrepresented groups, and research opportunities for undergraduate and graduate students.

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

Summary Statement

This project contains some challenging tasks and transformative concepts. The novelty of their proposed scientific approach is well elaborated. The broader impact on outreach is strong. However, it seems to lack of insights into fundamental physics or mathematics. In summary, I place the proposal among the top half among what I have reviewed.