Proposal Review 3 : 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:	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 proposal suggests developing a numerical simulation of self-assembling amphiphilic particles in solvent using the intuitive PDE relations instead of more computationally intensive molecular dynamics. The modeling is based on phenomenological models of amphiphiles in a solvent; these models describe aggregations of Janus particles and bilayers.

While this investigation could be important for organic chemistry, the proposal does not mention significant mathematical novelties and justification of the used intuivite model. The proposal mentions improving large-scale computations, but again few details are provided.

The plan is detailed, but it consists of listing the problem to be addressed, much less the means of the investigation.

The PI has a record of publications in this area, and he successively worked on the prior NSF-funded research.

The resources are adequate.

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 includes the advances in the simulation of collective self-assembling aggregates.
The PI proposes to work with several undergraduate students.

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

n/a

Summary Statement

The topic of the proposal is important and timely. The intuitive PDE dependence and the specific form of the potentials could be better justified.
I rank this proposal in the bottom third of the proposals I reviewed for this panel.

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