# Proposal Panel 1 : 2206369

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Agency Name: National Science Foundation

Agency Tracking Number: **2206369**

## Panel Summary

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BRIEF SUMMARY OF THE PROJECT:

The proposal describes a continuum model of self-assembling amphiphilic particles in a solvent. The model introduces an order parameter that minimizes a Ginzburg-Landau type energy. The aims of the proposed research is to extend the model to incorporate a double-well potential; develop a novel numerical method to solve it; and explore the effect of external forces on the self-assembly.

INTELLECTUAL MERIT:

Strengths: The panel found the problem interesting. The use of integral equations to solve the Allen-Cahn and hydrodynamic interactions was regarded as a strength. Another strength was the way the model accounted for small scales without resorting to molecular dynamics.

Weaknesses: When particles are almost touching the integrals become near-singular. The accurate evaluation of integrals in this case becomes an issue, but is not addressed in sufficient detail. It was also not clear how many particles the algorithm would be able to simulate and whether the algorithms could be scaled up to handle large numbers of particles. The proposal would have benefited from more specificity as to what kinds of flows, i.e., external boundary conditions, will be considered. The panel noted that including the study of the relation of the model parameters f(u) and g to experimental conditions, and that the addition of more details on the specific roles of each PI in the collaboration would have made the proposal more compelling. The proposal would have also been strengthened if further discussion on how to address these issues using mathematical analyses had been included.

BROADER IMPACTS:

The proposal involves the training of undergraduates, a graduate student, and possibly some high school students. The panel viewed this as a strength.

Results of Prior NSF Support:

The panel regarded results of prior NSF support as adequate.

Data Management Plan:

Adequate

Recommendation:

The panel appreciated the originality of the model, which includes its simplicity compared to molecular dynamics, as well as its potential ability to capture the behavior of real systems. However, there was insufficient detail to assess the feasibility of large scale simulations, and the proposal would have benefited from more extensive discussion of mathematical analysis of the model.

The panel placed the proposal in the Competitive category.

The summary was read by/to the panel and the panel concurred that the summary accurately reflects the panel discussion.

**PANEL RECOMMENDATION:** Competitive

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