

**MISSISSIPPI NSF EXPERIMENTAL PROGRAM TO STIMULATE COMPETITIVE RESEARCH
(MS EPSCoR)
MODELING AND SIMULATION OF COMPLEX SYSTEMS
COMPUTATIONAL CHEMISTRY GRANT PROGRAM FOR
MISSISSIPPI PREDOMINANTLY UNDERGRADUATE INSTITUTIONS
2013**

Deadline: July 20, 2013

BACKGROUND

The 2009-2014 Mississippi EPSCoR award from the National Science Foundation (NSF) Experimental Program promotes research in Modeling and Simulation of Complex Systems. One of the three research focus areas within this grant is computational chemistry (CompChem). The overall grant provides support for one research grant per year for a faculty member from a Mississippi Predominantly Undergraduate Institution (PUI) to perform collaborative research with EPSCoR computational chemistry faculty members.

COMPUTATIONAL CHEMISTRY PUI RESEARCH GRANT OBJECTIVES

The PUI grant is designed to encourage a PUI faculty member to collaborate on computational chemistry research with researchers at Mississippi research universities, to encourage undergraduate research in computational chemistry at the PUI, and to encourage students to pursue graduate education in computational chemistry or a related field. The research universities are Jackson State University, Mississippi State University, the University of Mississippi (including the University of Mississippi Medical Center), and the University of Southern Mississippi. The PUI grant is for one year. All research must be tightly integrated with core goals of the Mississippi NSF EPSCoR CompChem research focus area. Applicants are encouraged to read the description of the 2009-2015 NSF EPSCoR project at: <http://www.msepscor.org/> prior to submission to ensure that the proposed project is consistent with the objectives of the NSF EPSCoR grant. Applicants are also encouraged to contact Dr. Keith Walters, Science Coordinator, and/or Dr. Greg Tschumper, Computational Chemistry Research Focus Leader, to discuss the proposed research prior to submission (see contact information below).

ELIGIBILITY

Faculty members at any Mississippi institution designated as a PUI by NSF are eligible to apply. The proposed research must be integrated with the goals of the project as described at <http://www.msepscor.org/> and must be in collaboration with one or more senior personnel on the current project (see list below). Proposals for continuing grants in subsequent years will be considered.

FUNDING AMOUNT

Funding for each proposal is for one year and will not exceed **\$25,000** including F & A, pending availability of funds from NSF. Proposers should use the appropriate F & A rate for their institution.

COST SHARING REQUIREMENT

NSF EPSCoR funding requires cost sharing of 20% of total NSF costs. The cost share must meet NSF cost share requirements and cannot include any federal funds. Cost share will be the responsibility of the PUI researcher's home institution.

REPORTING REQUIREMENTS

Grantees are required to submit a final report (1-3 pages) within 2 months of the end of the grant period. The report should detail the activities, publications, extramural grant application(s), and/or extramural grant awards arising from this support. Include names, degrees and demographic information for any coworkers supported by the award. A reminder will be sent 1 month before the report is due.

FORMAT OF PROPOSAL

Applications should be prepared with the following specifications:

Page Size: 8 ½ x 11 inches, Spacing: Single, Font: Times New Roman or Arial, 12 point, Margins: 1”.

1. Cover Page (1 page)

- a. Proposal Title
- b. Principal Investigator (Full name, Title, Primary Affiliation, Office Phone Numbers and Cell Phone Number, Fax Number, E-mail Address)
- c. EPSCoR collaborator(s) (Full name, Title, Primary Affiliation, Office Phone Numbers and Cell Phone Number, Fax Number, E-mail Address)

2. Proposal (Maximum of 3 pages)

- a. Overview, objectives, significance, relevance to NSF EPSCoR computational chemistry research. (~1 page)
- b. Research plan and expected results—include a description of the nature of the proposed work and a publication plan (~1 page).
- c. Describe the nature of proposed collaboration with ongoing EPSCoR research activities. (~0.5 page)

3. Budget

All budgets are to be submitted in NSF format (1 page in NSF format for the funds being requested and another page in NSF format detailing the cost sharing). Budgets may include faculty salary, undergraduate student salary, fees, tuition, supplies, contractual, equipment and travel. The budgets must include appropriate fringes on all personnel salary. No subcontracts are allowed.

4. Appendices

- a. Budget justifications (1 page for NSF budget and one page for Cost Sharing)
- b. Curriculum vitae of PI (NSF biosketch format, 2 pages maximum). The biosketch should include a list of current and former undergraduate researchers. In the list of publications, place an asterisk next to the names of undergraduates co-authors.
- c. Statement agreeing to provide a final report and to present the research results at the Mississippi EPSCoR Annual Meeting (1 page).

PROPOSAL REVIEW

Proposals will be reviewed by the Principal Investigator (Dr. Sandra Harpole), Science Coordinator (Dr. Keith Walters), Computational Chemistry Research Focus Leader (Dr. Greg Tschumper), and rotating Computational Chemistry Steering Committee member. Criteria to be considered are scientific merit, relevance to MS EPSCoR's aims, budget justification, training opportunities for undergraduate students and potential for external funding.

SUBMISSION PROCEDURE, DEADLINE AND NOTIFICATION OF AWARD

Proposals should be contained in a single PDF file and sent as an email attachment to:

Dr. Keith Walters
Science Coordinator
Modeling and Simulation of Complex Systems
Mississippi NSF EPSCoR Program
Mississippi State University
Email: walters@me.msstate.edu
Tel: 662-325-8231

Deadline: July 20, 2013

Notification: August 1, 2012

Start Date for Proposals: September 1, 2013

Period of Performance: September 1, 2013 through August 31, 2014

Proposers are strongly encouraged to contact the Mississippi EPSCoR Science Coordinator or the Computational Chemistry Lead Investigator for additional information:

Computational Chemistry Lead Investigator

Dr. Greg Tschumper
Department of Chemistry and Biochemistry
University of Mississippi
Email: tschumpr@olemiss.edu
Tel: 662-915-5331

Other Computational Chemistry Researchers

Dr. Glake Hill
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Dr. Jerzy Leszczynski
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