IU BLOOMINGTON

EMERGING AREAS OF RESEARCH

Abstract Template -- Due June 30, 2017

Title of initiative to be proposed:

EAR: Environmental and Materials Chemistry Modeling Consortium [E-MC2]

Name of lead PI, with title, department/school:

Srinivasan S. Iyengar, Associate Professor, Department of Chemistry, Adjuct in Physics, COAS

Key team member names and departments/schools (up to 10 names):

coPIs: Krishnan Raghavachari (Chemistry), Peter Ortoleva (Chemistry, Informatics (Adjunct)), Vikram Jadhao (Intelligent Systems Engineering, Informatics)
Senior Personnel: Chemistry: Phil Stevens (SPEA), Liang-shi Li (Chemistry), Caroline Jarrold (Chemistry), Sara Skrabalak (Chemistry), Amar Flood (Chemistry), Jeremy Smith (Chemistry)

Description of area to be proposed. What constitutes this area of research or creative activity as emerging? (Word limit=500)

Rationale and Strength

Theoretical and computational chemistry is central to the materials genome initiative and impacts the design of new catalysts, vaccines, nanoparticle therapeutic delivery systems, and understanding environmental chemistry. The complexity of the systems requires sophisticated approaches in theoretical chemistry. True advances are limited by lack of quantitative predictive models because accurate treatment of such systems is an exponential scaling high-performance computing problem.

Since the 1960s, through efforts from Harrison Shull, Donald McQuarrie, and Ernest Davidson, (all IU Bloomington) has been prominent in the development and application of new computational methods. Examples of IU's influence include (a) the Quantum Chemistry Program Exchange that allowed storage of, and global access to, a repository of computer programs and chemical information, and (b) state-of-the-art computing facilities that have been a constant resource and support for the community.

Targeted Outcomes

This initiative will allow fundamental developments and new predictive technologies that harness our existing and proven capabilities in (a) quantum mechanical computations, (b) multiscale theoretical quantum dynamical theory and multistate computational statistical mechanics, (c) continuum electrostatics and its interface with atomistic simulations, (d) new algorithm development, and (e) deciphering patterns in large data-sets generated from our studies through interfacing with machine learning.

The new methods we develop will, in collaboration with listed senior personnel, deliver new insights and paradigm shifts in environmental, nanomedical, and materials science. These will include the following: (a) novel custom synthetic solutions to artificial nitrogen fixation, (b) molecular-level understanding of chemical drivers of climate change, air pollution, and nutrient cycling, (c) electron transport in photovoltaic devices, organic and optoelectronic devices, OLEDs and sensors, (d) nanoparticle vaccine design and therapeutic delivery systems, (e) nanoparticle nucleation, self-assembly and plasmonics.

Future Directions

The investigators listed have a track record of external funding (NSF, NIH, DOE). This initiative will build on existing strengths, produce new directions and lead to external grants in support of center activities.

Please submit to earprogram@indiana.edu