RX21-2

1. **Research Title:** Molecular simulation of enzyme-substrate complexes.

2. **Individual Sponsor:** List the AFRL research topic sponsor's contact information

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3. **Academic Area/Field and Education Level**
Chemical Engineering/Chemistry/Bioengineering/Materials Engineering/Materials Science (MS or PhD level)

4. **Objectives:** Investigate enzyme-substrate complexes via atomistic simulations.

5. **Description**: The project will utilize multiscale modeling techniques ranging from QM, QM/MM, and MD, to coarse-grain models in order to investigate the structure and binding energetics of enzyme-substrate complexes. *De novo* structure predictions will be utilized if needed to determine the 3-D structure of the complexes. Close ties with the bioinformatics and synthetic biology research groups will be fostered in order to guide in the development, design and rapid screening of enzyme-mutations for enhanced performance. The project aims to address areas of significant impact to US DoD and in particular aerospace interests such as bio-sequestration of valuable metals and biodegradation of environmental pollutants.
(QM=quantum mechanics; MM=molecular mechanics; MD=molecular dynamics).

6. **Research Classification/Restrictions:** This research is unclassified and has no restrictions.

7. **Eligible Research Institutions:** Ohio research universities that offer graduate level research programs in the disciplines listed above.

**NOTE: Topics submitted to DAGSI must be approved for public release. Need PA Approval #**