SEMS: RESEARCH PROJECT DESCRIPTION

1. Project Background and Description

Project title:
Liquid Biofuel Property Predictions using Molecular Dynamics Simulations

Project description:
The overall aim of this study is to predict the physicochemical properties of combustion of liquid biofuels (such as bioethanol and biodiesel) and their blends using Molecular Dynamics (MD) simulations. The high-fidelity MD simulations will reveal the details of combustion of these renewable fuels and fuel blends, obtaining an in-depth understanding on the combustion characteristics including chemical kinetic pathways and mechanisms of pollutant formations.

2. Project Scope

The main objectives of the project are:

1) To develop a Molecular Dynamics (MD) simulation model to understand the reaction kinetics of liquid biofuel combustion.
2) To gather an in-depth understanding on the combustion utilisation of liquid biofuels in engines including pollutant emissions.
3) To validate the MD simulation results and publish the research outcomes in leading journals.

3. Desired Skills from the Student

The successful applicant needs to have strong analytical, computational and mathematical skills, with academic background in Engineering Science (such as Chemical Engineering, Mechanical Engineering, or Aerospace Engineering), or Physical Science, or Chemistry, or Mathematics.

The applicant needs to have an interest in Energy research, and an aspiration of becoming an independent researcher with own initiatives.

Programming skills are desirable (but not essential at this stage) for the project research. Effective communication skills are essential.

4. Supervisory Team

Primary: Professor Xi Jiang
Secondary: Professor Teresa Alonso-Rasgado