

|| SEMS: RESEARCH PROJECT DESCRIPTION

1. Project Background and Description

Project title:

Molecular Dynamics Simulations of Pollutant Formation in Combustion Engines

Project description:

The overall aim of this study is to predict the pollutant formation (e.g. soot particles and PM2.5) in combustion of hydrocarbon fuels for applications such as marine diesel engines using Molecular Dynamics (MD) simulations. The high-fidelity MD simulations will reveal the details and mechanisms of pollutant formation, obtaining an in-depth understanding on the pollutant formation process including chemical kinetic and physical pathways. Developments of new models will also be attempted.

2. Project Scope

The main objectives of the project are:

- 1) To develop a Molecular Dynamics (MD) simulation model to simulate diesel/biodiesel combustion and soot formation.
- 2) To gather an in-depth understanding on the chemical kinetic and physical pathways in the formation processes of soot particles and PM2.5.
- 3) To develop physicochemical models for the formation processes of soot particles and PM2.5 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**