



**Postdoctoral Appointee - Theoretical Chemical Kinetics and Chemical Kinetic Modeling**  
**Chemical Sciences and Engineering**  
**Requisition #416135**

**Job Description**

The Chemical Sciences and Engineering Division is seeking a Postdoctoral Appointee for the development and/or application of theoretical chemical kinetics and chemical kinetic modeling to the study of gas-phase chemical reactions. The theoretical predictions will be used to guide the development of coupled kinetic models with a view to interpreting chemically reacting systems at high temperatures or highly energized/non-thermal environments. A particular emphasis will be on the unimolecular and bimolecular kinetics of molecules relevant to combustion and atmospheric processes.

The project will support effort in one of the following areas:

- (1.) Applications of in-house theoretical kinetics tools to develop and interpret detailed coupled kinetics models and/or
- (2.) The development of new dynamical theories, computational strategies, and high-performance computing software, as well as the application of semiclassical dynamics and transition state theory to characterize pressure-dependent and many-body chemistry.

Perform theoretical calculations of the electronic structure and chemical kinetics for combustion/atmospheric chemistry relevant reactions. Ability to use and/or develop in-house kinetics and UQ tools for interpreting coupled kinetics models to describe gas phase reactivity.

**Position Requirements**

- This level of knowledge is typically achieved through a formal education in physical chemistry or chemical/mechanical engineering at the Ph.D. degree level with zero to three years of experience or equivalent in the scientific application of this knowledge and practical laboratory experience
- Considerable experience in at least one or more of the following areas: electronic structure theory, theoretical chemical kinetics and/or theoretical chemical dynamics, combustion/atmospheric chemistry
- Good knowledge of gas phase chemical kinetics, chemical physics, physical chemistry, combustion/atmospheric chemistry
- Communicates effectively with the supervisor, peers and laboratory management through research reports, project presentations and other regular channels
- Maintains comprehensive knowledge of pertinent literature
- Develops new ideas, concepts, and/or research proposals to create programmatic growth and intellectual property for the Division
- This position description documents the general nature and level of work but is not intended to be a comprehensive list of all activities, duties and responsibilities required of job incumbent. Consequently, job incumbent may be required to perform other duties as assigned

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