



**Postdoctoral Appointee - Chemical Kinetics
Chemical Sciences and Engineering Division
Requisition # 417220
Lemont, Illinois**

Job Description

The Chemical Sciences and Engineering Division at Argonne National Laboratory is seeking a postdoctoral appointee whose effort will be devoted to 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 in complex systems such as in combustion, atmospheric processes, or in sustainable energy conversion/manufacturing processes.

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

- (a) Applications of in-house theoretical kinetics tools to characterize gas phase reactivity in molecular systems across the periodic table and/or
- (b) develop and interpret detailed coupled kinetics models to predict reactivity in sustainable energy conversions.

Perform theoretical calculations of the electronic structure and chemical kinetic modeling for combustion/atmospheric/sustainable-energy-conversion 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. 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.

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, kinetics modeling, 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, energy conversion processes
- 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
- Ability to model Argonne's Core Values: Impact, Safety, Respect, Integrity, and Teamwork

Please click on the link to apply:

[ARGONNE CAREERS \(myworkdayjobs.com\)](https://myworkdayjobs.com/Argonne)