



The Combustion Institute

5001 Baum Boulevard, Suite 644
Pittsburgh, Pennsylvania 15213-1851
USA
Ph: (412) 687-1366
Office@CombustionInstitute.org

Fax: (412) 687-0340
CombustionInstitute.org

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Postdoctoral Position: Rocket Combustion Studies at the Air Force Research Laboratory

Our research centers on fundamental chemical kinetics and applications in combustion chemistry of energetic propellants. The rates of elementary reactions are measured using various direct time-resolved techniques such as pulsed laser photolysis, coupled with laser-spectrometric or mass-spectrometric probing of the short-lived species in the gas phase. We also use rapid-scan FTIR absorption spectroscopy to probe the formation of stable products in these reactions. Heterogeneous processes, such as the reactions of aerosolized propellant fuel in various oxidizing gaseous environments, are studied using the VUV-PI-TOFMS experimental set-up of the Chemical Dynamics Beamline 9.0.2.3 at the Advanced Light Source Synchrotron Facility at the Lawrence Berkeley National Laboratory in Berkeley, CA.

High level quantum chemistry approaches, which include *ab initio* multi-reference second-order perturbation, quadratic configuration interactions, and coupled-cluster theories, as well as density functional theory, are applied to ascertain the nature of the potential energy surface and the reaction dynamics involved. Rice-Ramsperger-Kassel-Marcus theory is applied and multi-well master equation simulations carried out to compute the P-T dependences of the reaction rate coefficients. Efficient methods in direct *ab initio* molecular dynamics simulations are being developed for *a priori* construction of reduced reaction mechanism sets to aid not only the above computations and experiments, but also computational fluid dynamics simulations of the chemistry occurring in real propulsion/combustion devices and space environments.

Terms:

- (1) Tenure of up to two years
- (2) NRC research associateship stipend rate applies

Requirements:

US citizenship
Ph.D. in Chemistry, Physics, or Aerospace Sciences
Strong background in spectroscopy, *ab initio* electronic structure theory, or numerical recipes
Exemplary research publication record
Demonstrated leadership in project management
Teaming skills

Desired:

Demonstrated experience in time-resolved measurement techniques
Working knowledge of high-T, high-P, and high-vacuum experimental apparatuses
Demonstrated skill in using MOLPRO, VeriFlex, GAMES, or CHEMKIN-PRO

To apply:

(1) Email CV to Dr. G. L. Vaghjani at: ghanshyam.vaghjani@us.af.mil

(2) For detailed instructions visit:

[http://nrc58.nas.edu/RAPLab10/Opportunity/Opportunity.aspx?LabCode=13&ROPCD=133003
&RONum=B7679](http://nrc58.nas.edu/RAPLab10/Opportunity/Opportunity.aspx?LabCode=13&ROPCD=133003&RONum=B7679)

To learn more about the Air Force Research Laboratory:

Visit: <http://www.wpafb.af.mil/afri/rq/>

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