Opportunity Title: Computational High-Temperature Sensing Materials
Opportunity Reference Code: NETL-2019-PGRP-Duan-1

Organization National Energy Technology Laboratory (NETL)

Reference Code NETL-2019-PGRP-Duan-1

How to Apply A complete application consists of:

- An application
- Transcripts – Click here for detailed information about acceptable transcripts
- A current resume/CV, including academic history, employment history, relevant experiences, and publication list
- Two educational or professional references

All documents must be in English or include an official English translation.

If you have questions, send an email to NETLinfo@orau.org. Please include the reference code for this opportunity in your email.

Application Deadline 8/1/2019 11:59:00 PM Eastern Time Zone

Description Through the Oak Ridge Institute for Science and Education (ORISE) this posting seeks a post-doctoral researcher to engage with National Energy and Technology Laboratories (NETL) teams on the development of high temperature gas sensors for power generation and industrial applications, such as combustion processes, solid oxide fuel cells (SOFCs), aerospace and metal refining industries, which is essential to improve energy efficiency and reduce toxic emissions. However, gas sensors operating at high temperatures encounter many challenging issues, such as thermal shock resistance and long-term stability, sensitivity, reproducibility and selectivity. Solid-state gas sensors operate based on the interaction of sensing materials with the surrounding environment resulting in modifications to the electrochemical potential, the resistivity, the density, and/or the optical properties. Gas adsorption processes relevant for high-temperature operation must show chemical binding energies larger than the thermal energy kT and the bulk reactions begin to play a significant and, in some cases, dominant role in sensing responses at high temperatures. Sensing processes at such high temperatures are complicated and not well understood, so theoretical modeling is needed to explore high-temperature gas sensor mechanisms and support development of practical sensor devices.

To continue our previous research (Wu *et al*, **J. Phys. Chem. C**122(2018)22642-49), in this study, the atomistic-level simulations (DFT, MD/MC) will be applied and combined with thermodynamic and optical / electronic property modeling to investigate the sensing mechanisms of functional oxide materials in high temperature gas streams relevant for advanced energy conversion systems. Through close collaboration with in-house experimental teams, the focus of this research and learning opportunity for the candidate will be on i) thermodynamic, electronic and optical properties of pure, defective and doped sensor materials at high temperature through electron-phonon interaction and thermal expansion; ii) gas molecules interacting with pure and defective surfaces of sensor

materials; iii) gas sensor pathways and corresponding kinetics; iv) selectivity and stability of sensor materials when sensing gases; and v) improving sensitivity and selectivity by creating defects and doping.

Qualifications

- The successful candidate will possess demonstrable skills in advanced computational methods (DFT, *ab initio* MD/MC, lattice phonon dynamics) for solving complex problems. The successful candidate will possess significant experience in fundamental research on electronic and optical properties of solids, and will preferably have experience in programming suitable for a high performance computing environment (e.g. parallel processing and programming in MPI environment). The successful candidate will possess excellent communication skills, and will possess demonstrable experience completing research in a collaborative/team environment. The successful candidate is not required to possess specific experience in sensor development, but preference will be given to candidates with experience in sensors, solid oxide fuel cells, electroceramic materials, electrochemistry, and other energy conversion devices.
- All applicants should possess a doctorate degree in physics, material science, chemistry, or a related discipline, with experience and publications in density functional theory, molecular dynamics, Monte Carlo simulations.

Eligibility Requirements

- **Degree:** Any degree .
- **Discipline(s):**
  - **Chemistry and Materials Sciences** (12 👁)
  - **Communications and Graphics Design** (2 👁)
  - **Computer, Information, and Data Sciences** (16 👁)
  - **Earth and Geosciences** (21 👁)
  - **Engineering** (27 👁)
  - **Environmental and Marine Sciences** (14 👁)
  - **Life Health and Medical Sciences** (45 👁)
  - **Mathematics and Statistics** (10 👁)
  - **Other Non-Science & Engineering** (2 👁)
  - **Physics** (16 👁)
  - **Science & Engineering-related** (1 👁)
  - **Social and Behavioral Sciences** (27 👁)

Affirmation I certify that I:

- Have an earned or will receive a doctoral by appointment start date.

OR

- Have received the degree no more than five years before the date of application (postdoctoral applicants).