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| **TITLE:** | Computational High-Temperature Sensing Materials |
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| **DEPARTMENT:** | U.S. Department of Energy/National Energy Technology Laboratory (NETL) |
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| **NETL CONTACT:** | Dr. Yuhua Duan, yuhua.duan@netl.doe.gov |
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| **DUTY LOCATION:** | Pittsburgh, PA |

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| **ACADEMIC LEVEL:** | **x** | PhD |  | MS |  | BS |  | Undergrad |  | Faculty |

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| **POSITION** **INFORMATION:** | 1-year appointment; full time (40 hours per week) with the possibility of extension |
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| **CLOSING DATE:** | August 1, 2019 |
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| **WHO MAY BE** **CONSIDERED:** | United States Citizens, LPRs, & Foreign Nationals with appropriate approval which includes F-1 OPT with EAD (STEM extension not valid), J-1 Exchange Visitor, and LPR with EAD |

**SUMMARY:**

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, 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 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.

**Key qualifications for the post-doctoral research position:**

* 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. The appointment will be administered through the Oak Ridge Institute for Science and Education (ORISE), which requires applicants to have obtained their Ph.D. within the past five years.

**HOW TO APPLY:**

Applicants should apply through the Oak Ridge Institute for Science and Education (ORISE) program. The ORISE program provides opportunities for undergraduate students, recent graduates, graduate students, postdoctoral researchers, and faculty researchers to apply classroom knowledge in a real-world setting to learn about NETL’s core mission areas.

* Interested applicants should complete the online application at http://www.zintellect.com. For questions or issues, please email NETLadmin@orau.org.
* In the online application, **list** **Dr. Yuhua Duan as your requested mentor.** This will associate your application with this research opportunity. Please send a CV to yuhua.duan@netl.doe.gov.
* If you have additional questions, please contact Patricia Adkins-Coliane, Patricia.adkins-coliane@netl.doe.gov, who is the NETL Graduate Education Program Manager.

The participant(s) will be assigned to the program solely for the educational benefit it provides. The assigned project should not include activities that are reserved for federal employees nor should it require a participant to perform inherently governmental functions such as: supervise or mentor federal employees or federal contractor staff, hire or fire anyone; have budget, program management, or signature authority; carry an official job title; or function in any way as a representative of the federal government.