**TITLE:** Computational Chemist / Physicist / Materials Scientist / Electrochemist
**DEPARTMENT, AGENCY:** Department of Energy, National Energy Technology Laboratory
**STIPEND RANGE:** Depends on level of experience
**OPEN PERIOD:** Open until filled
**LEVEL:** Post-Doctoral Research Associate (preferred), Faculty (preferred),or Graduate Student
**POSITION INFORMATION:** Temporary Appointment: 1 year period between approximately June 1, 2015 and May 30, 2016; Full-Time (40 hours per week); multiple appointments possible
**WHO MAY BE CONSIDERED:** United States Citizens and Foreign Nationals with approval

## DESCRIPTION:

An opportunity exists for post-doctoral researchers to develop computational models and data analysis tools to support NETL Solid Oxide Fuel Cells research. Research efforts focus primarily on: (1) accurate capture and computational representation of relevant physical and chemical processes; and (2) validation of models using detailed in-house experiments or independently published reports. Among individual model development tasks, priority has been assigned to ensure that the models and tools are computationally efficient, widely accessible, and share data among discrete modules. This position will provide support to transfer existing models to a High Performance Computing (HPC) platform, operate the codes to ensure accurate results are being obtained, apply user interfaces on models to facilitate broader accessibility, and integrate component models. Broadly, the project goals are:

1) Generate, enhance, and increase efficiency of fuel cell component models using commercially relevant codes and techniques to facilitate rapid execution;
2) Establish a user interface for independent fuel cell models to permit a novice simulator to complete relevant simulations;
3) Implement a methodology for data exchange between independent modules, ultimately producing a comprehensive SOFC performance model;
4) Ensure that models utilize efficient computational methods, including computations in true parallel fashion;
5) Generate high fidelity visualization tools supporting analysis.

## SPECIFIC TASKS:

The specifically envisioned tasks support the broad goals described above, and may include one or more of the following elements.

1) Examine existing high performance codes to ensure proper operation, fidelity of data output, and suitability for integration. The priority ranking for examination of the codes:
    a. Oxygen Reduction Reaction Model (Reaction Electrochemistry, Electroceramic Transport)
        - General Description: Multivariable dynamic 1-D model
        - Time domain: seconds
        - Length domain: microns
        - Programming: FORTRAN
    b. 3D Multi-Physics Model (Computational Fluid Dynamics, Reaction and Transport)
        - General Description: Multivariable dynamic 3-D model
        - Time domain: seconds
        - Length domain: multi-micron to centimeters
        - Programming: FORTRAN, COMSOL
    c. Microstructural Evolution Model (Phase Field Modeling)
        - General Description: Multivariable dynamic 3-D phase field model
        - Time domain: seconds to k-hrs
        - Length domain: microns to millimeters

- Programming: FORTRAN

d. Diffuse Interface Model (Phase Field Modeling)
   - General Description: Multivariable dynamic 1-D and 3-D phase field model
   - Time domain: seconds to k-hrs
   - Length domain: nanometers
   - Programming: FORTRAN

e. Surface and Interface Property Modeling
   - General Description: ab initio modeling
   - Time domain: sub micro-second
   - Length domain: nanometers
   - Programming: VASP

f. High Fidelity Impedance Model (Dynamic Reaction and Transport Modeling)
   - General Description: Multivariable dynamic 3-D model
   - Time domain: seconds
   - Length domain: multi-micron to centimeters
   - Programming: FORTRAN, COMSOL

g. Bayesian Statistical Model (Statistical Methods and Modeling)
   - General Description: Statistical Model
   - Time domain: N/A
   - Length domain: N/A
   - Programming: MATLAB, FORTRAN

2) As necessary, generate stand-alone computational modules that allow rapid computing. Models should contain a user interface that allows manipulation of parameters by a non-expert user. Results generated using the HPC environment must be compared to those generated via PC, to ensure equivalency of the computing environments.

3) Integrate phenomenological models to create higher-order computational tools and resources. Generate methods to pass data from one computational module to another in the HPC environment, such that results from one model can be used to update the starting parameters in another model. Ensure that the models can all be executed in true parallel form.

4) Generate high quality visualization tools indicating cell performance in time and space. Permit user queries at high fidelity.

Examples of SOFC modeling completed by NETL researchers are embodied in the following references:

Linyun Liang, Qun Li, Jiamian Hu, Shiwoo Lee, Kirk Gerdes, and Long-Qing Chen, “Phase field modeling of microstructure evolution of electrocatalyst-infiltrated solid oxide fuel cell cathodes,” Journal of Applied Physics 117, 065105 (2015)

Jia-Mian Hu, Linyun Liang, Yanzhou Ji, Liang Hong, Kirk Gerdes, and LongQing Chen, “Interdiffusion across solid electrolyte-electrode interface,” Applied Physics Letters 104 21 (2014) 213907

Hui Zhang, Mingyang Gong, Kirk Gerdes, and Xingbo Liu, “Surface Transport Mechanism and Bi-Pathway ORR Kinetics for Solid Oxide Fuel Cell Cathode,” J Electrochemical Society 161 (10) F983 (2014).

S. Raju Pakalapati, Kirk Gerdes, Ismail Celik, Harry Finklea, Mingyang Gong, and Xingbo Liu, “Micro-Scale Dynamic Modeling of LSM/YSZ Composite Cathode” Solid State Ionics 258 (2014) p45.

## **QUALIFICATIONS**:

The successful candidate will possess demonstrable skill in advanced mathematical algorithms and computational methods for solving complex reaction and transport problems. The successful candidate will possess significant experience in identified computer programming, 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 solid oxide fuel cells, but preference will be given to candidates with experience in solid oxide fuel cells, electroceramic materials, electrochemistry, or any related systems in sensors, membranes, and other energy conversion devices. Programming languages and applications codes mentioned are those expected in the project though it is not necessary to have experience using a specific application code/programming language; general experience and the ability to quickly adapt application code/language is acceptable.

Interested candidates may contact Dr. Kirk Gerdes (kirk.gerdes@netl.doe.gov) directly with a current CV at the earliest opportunity.

## HOW TO APPLY:

Applicants should apply through the Oak Ridge Institute for Science and Education (ORISE) program (orise.orau.gov). NETL utilizes the ORISE program to support research and work within NETL's Office of Research & Development.

• Interested applicants should complete the online application at http://www.orau.gov/netl/
• In the online **application list one of the following as your requested mentor** to associate your application with this job posting.

Dr. Kirk Gerdes

Dr. Vyacheslav Romanov
- 3D Multi-Physics Model
- High Fidelity Impedance Model
- Bayesian Statistical Model

Dr. Dan Sorescu
- Microstructural Evolution Model
- Diffuse Interface Model
- Surface and Interface Property Modeling

Dr. Paul Ohodnicki
- Oxygen Reduction Reaction Model

If you have additional questions please contact the NETL ORISE program coordinator, Nancy Andres, Nancy.Andres@NETL.DOE.GOV.