

Job opening for Computational and Theoretical Chemistry Program Manager

The Office of Basic Energy Sciences (BES) within the Office of Science in the Department of Energy (DOE) is seeking an individual (US Citizenship required) to manage a portfolio of fundamental research focused on Computational and Theoretical Chemistry (CTC) in the Fundamental Interactions Team, within the Chemical Sciences, Geosciences, and Biosciences Division. This is a permanent position located in Germantown, Maryland and the successful applicant will become a Federal employee under the GS pay and benefit system. The job title is Physical Scientist (GS 15) with a pay range of \$137,849 - \$166,500. This position is to be filled under the OPM Government-Wide Direct Hire Authority Certain STEM Positions. An Appointment made with this authority may be processed as a new appointment into the Civil Service. The incumbent may be required to serve a mandatory one (1) year probationary period. This position may be designated as a Testing Designated Position (TDP) and subject to testing for illegal drug use. Additionally, a preliminary background check must be completed before a new employee can begin work. All positions are subject to satisfactory security and suitability determinations.

Duties

The Physical Scientist will determine scientific focus and direction of the CTC research program, prepare calls for proposals, organize independent peer reviews, recommend funding allocations, organize Principal Investigator meetings, serve as a liaison on committees, and assess scientific progress of the program. The CTC program manager conceives, justifies, plans, initiates, manages, and coordinates all aspects of the program that includes a diverse range of theoretical and computational research projects in chemical and physical sciences. Areas of current interest include, but are not limited to: Development and integration of new and existing theoretical and massively parallel computational approaches for the deterministic, accurate, and efficient prediction of chemical and physical processes and mechanisms; efforts aimed at enhancing the accuracy, precision, and applicability or scalability of quantum-mechanical simulation methods; development of spatial and temporal multiscale methodologies to allow time-dependent simulations of resonant, non-resonant and dissipative processes as well as rare events; development of capabilities for simulation of light-matter interactions; conversion of light to chemical energy or electricity; ability to model and control externally driven electronic and spin-dependent processes in real environments; development of novel approaches to apply data science tools (e.g., machine learning) to advance the discovery of emergent phenomena in chemical and physical processes; and advances of computational approaches to exploit emerging quantum computers to solve currently intractable problems in chemistry and physics.

Qualifications

Applicants must have one year of experience at a level of difficulty and responsibility equivalent to the GS-14 grade level in the Federal service. Such experience includes evaluating the effect of technical developments on fundamental policies, objectives and goals; developing new concepts, planning, and evaluating long-range programs and projects; planning and executing specialized programs on scientific, technical, administrative, and fiscal matters; and/or developing and managing funding for scientific research programs, determining funding levels, and recommending proposal, declinations and program determinations for assigned programs.

The successful candidate will be a scientist who is recognized for expertise in fundamental theories of molecular processes and the translation of this theory to computational approaches that advance BES research in chemistry and physics. S/he must have served as a major contributor or a Principal

Investigator on original scientific research project(s) that resulted in peer-reviewed, archival journal articles and invited presentations at national and international meetings. In addition, the candidate must have supervised original scientific research efforts of doctoral students, postdoctoral researchers, and/or junior staff. S/he must have previous experience in evaluating research, including proposals and research publications.

Additionally, experience should involve determining the scientific focus and direction of a scientific research program by preparing calls for proposals, organizing independent peer reviews, recommending funding allocations, monitoring scientific program progress, and reviewing, recommending, and declining research proposals. Experience should involve managing scientific research, such as developing and defending requests for funding within an organization and managing budgets and staffing for research project(s). Experience in effective communication of information orally and in writing is expected, such as presenting strategies, advisory opinions and recommendations to managers and supervisors, as well as to varied audiences in formal and informal settings.

This position has a positive education requirement. Therefore, you must provide documentation supporting any education claims in your application. This documentation can include unofficial transcripts or any report listing institution, course title, credits earned and final grade. For specific education requirements, please see the Education Requirements below. If selected, official transcripts will be requested. Education must be obtained from an accredited institution recognized by the U.S. Department of Education. Foreign education must be reviewed by an organization recognized by the U.S. Department of Education. For special instructions pertaining to foreign education and a list of organizations that can evaluate foreign education, see [the Department of Education website](#). In addition to the above-referenced experience, applicants must have one of the following to satisfy the basic requirements for this position:

- A. A degree in physical science, engineering, or mathematics that included 24 semester hours in physical science and/or related engineering science such as mechanics, dynamics, properties of materials, and electronics.

or

- B. A combination of education and experience – education equivalent to one of the degree listed in A (above) that included at least 24 semester hours in physical science and/or related engineering science, plus appropriate experience or additional education.

NOTE: OPM Qualification Standards for the GS-1301 series can be found at the following website: <https://www.opm.gov/policy-data-oversight/classification-qualifications/general-schedule-qualification-standards/1300/general-physical-science-series-1301/>

Applications

To be considered for this position, you must submit your application via email to Bruce.Garrett@science.doe.gov (with a carbon copy to Jeff.Krause@science.doe.gov) by 5:00 pm (EST) on Monday, December 16, 2019.

Applications for this position must include the following:

- A cover letter detailing previous experience relevant to the duties and qualifications required for a Program Manager position in Computational and Theoretical Chemistry
- A curriculum vitae with a complete list of publications
- Transcripts

Your application must describe how you meet the qualifications and how your past experience demonstrates that you possess the knowledge and abilities required to successfully perform the duties of this position. Transcripts can be submitted after the deadline but will be required before the application is considered.

Other information

More information about BES can be found at: <https://science.osti.gov/bes>. A complete description of the BES Computational and Theoretical Chemistry program can be found at: <https://science.osti.gov/bes/csgb/Research-Areas/Computational-and-Theoretical-Chemistry>. Details of the current research portfolio may be found in the abstracts of the most recent principal investigators' meeting at <https://science.osti.gov/bes/csgb/Principal-Investigators-Meetings>.

Interested applicants are strongly encouraged to contact Bruce Garrett (Bruce.Garrett@science.doe.gov), or Jeff Krause (Jeff.Krause@science.doe.gov) for more information about this position and the application process.