Clark Atlanta University
Job Description

Position Title:	**Staff Scientist / Research Computing Specialist**
Employee:	**To be hired**
Department:	**Department of Chemistry**
Reports To:	**Principal Investigator (Dr. Dinadayalane Tandabany)**

The following statements are intended to describe the general nature and level of work to be performed. They are not intended to be construed as an exhaustive list of all responsibilities, duties and skills required of personnel so classified.

General Function (Description):

This person will assist the Principal Investigator (PI, Dr. Dinadayalane Tandabany) with the inst619( )TffTc 001 T(en)-8 d.tenl software on workstations running on Windows and Linux operating systems, maintaining the software and hardware. The successful candidate will perform federally funded research with undergraduate and graduate students using computational chemistry including ab initio and DFT calculations and MD simulations. He/she should have strong technical knowledge of a wide range of computational and visualization software, for example, Gaussian 16, VASP, Gromacs, NAMD, LAMMPS, VMD, Spartan, Scigress, GaussView. Knowledge of coding using Python and/or R is required. He/she will work with undergraduate/graduate students in collecting and checking data for preparation of manuscripts. Also, this person will work with the Co-PI and/or collaborators associated with the project in collecting and checking data for preparation of collaborative manuscripts. He/she will also assist PI in preparation of manuscripts and successful submission to publication in the peer-reviewed journals. Furthermore, he/she will also keep the collected scientific data secure and train the students for data management by working with the Principal Investigator. The person hired for this position will be expected to adhere to Clark Atlanta University policies and procedures.

Examples of Duties and Responsibilities:

(1) Install software and manage the workstations, trouble shooting of software, installation of operating systems, and training of students are regular duties.
(2) Prepare tutorials for students on using the specific modules of the software and train them successfully by working with the PI.
(3) Assisting the PI for mentoring students and/or directly mentoring students as assigned by the PI in computational research projects funded by the federal agency.
(4) Prepare reports and work with the PI for dissemination of results by publications in peer-reviewed journals.
(5) Attending all the meetings with the project team and the collaboration meetings.
(6) Participate and learn in the workshop related to computational chemistry and molecular dynamics, data analytics, learning new techniques like Artificial Intelligence (AI) and Machine Learning (ML) as needed.

Knowledge, Skills and Abilities

The applicant should have the skills on current techniques and technology applied to computational chemistry and materials science. Knowledge of working with different operating systems including Windows, Linux, MacOS as well as supercomputers for running and installing software is required. Successful applicant should have knowledge by vast experience of using the techniques of ab initio, DFT and molecular dynamics (MD) simulations for research, data analysis, mentoring of undergraduate students, writing manuscripts and successful publications in peer-reviewed journals. Interpersonal and organizational skills are needed to work with students on computational and data intensive projects. Experience of coding using Python and/or R is required. This person should have skills to editing software of audio/video, import/export videos on YouTube; strong communication skills; interest to mentoring undergraduate students; very knowledgeable on Microsoft Office suites including word, PowerPoint, Excel, data plotting/graphing software, databases.