

*****Postdoc Position available*****

A new NSF-funded position is available for a post-doctoral scholar. The project is titled *Bridging electronic structure theory and dynamics with applications to nonadiabatic processes*. Work will involve development and application of interpolative methods (IMLS) for fitting potential energy surfaces (PESs). A main priority will be organizing and extending existing codes into a user-friendly distributable software package. Some information about our group and recent projects can be found on our webpage: <http://web.mst.edu/~dawesr/>

One avenue of this project (in collaboration with MCTDH developers) is to develop interpolative fitting in a sum-of-products form and directly interface to the MultiConfigurational Time-Dependent Hartree (Heidelberg) MCTDH code package. This could facilitate highly accurate and efficient quantum dynamics studies. We are currently studying systems of interest to atmospheric and interstellar chemistry in terms of their spectroscopy and dynamics. This also involves systematic studies of systems which include various non-adiabatic interactions between states such as conical intersections, Renner-Teller, and spin-orbit coupling to assess the importance of such effects.

A motivated individual can expect to develop a strong publication record, travel to conferences, and have opportunities to interact with university and national lab collaborators.

Qualifications:

- A recent PhD in chemistry or physics.
- Substantial experience with Fortran coding and scripting.
- Experience with multireference quantum chemistry and/or computational spectroscopy or dynamics and familiarity with the MCTDH package is an asset.

For more information please send an email with a detailed cover letter describing previous research experience, your CV, and a list of three references.



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