

## Ph.D. student (f/m/d) for predictive power in Materials Science

**Are you passionate about innovation? Do you love developing applied science with environmental impact? Do you use multidisciplinary thinking to solve professional questions? Are you able to appreciate the beauty of nature's answers to its many challenges? Would you like to innovate in an international and highly collaborative environment? Then the Chair of Biogenic Functional Materials (BFM) at the Technical University of Munich (TUM) is the perfect place for your future. BFM offers state-of-the-art infrastructure comprising three inter-disciplinary and inter-connected laboratories focused on the synthesis and engineering of biogenic and sustainable photo-electro-active materials, mechanical/spectroscopic/electrochemical characterizations, and the engineering of lighting and photovoltaic devices with researchers from around the world. We are located at the young TUM Campus Straubing, aiming to become the European leader in developing sustainable technologies and their economic implementation. Learn from Biology, think like a Chemist, and handle like an Engineer...are you ready?**

### *Mission*

We are looking for a motivated Ph.D. student with a solid background in theoretical chemistry and a strong motivation to develop new prediction tools for material science. The candidate, together with a multidisciplinary and cross-functional team will focus on the theoretical analysis and understanding of electronic/molecular structures (ground and excited states) along with the design, implementation, training and analysis of machine learning models towards the smart design of novel functional nanomaterials (e.g., coordination complexes, low-dimensional materials, hybrid materials, bio-hybrids, protein-based materials, etc.) for applications in energy conversion.

### *The successful applicant must have the following:*

- Master's Degree/(10-semester diploma) in chemistry or related disciplines.
- Strong background and proven experience in theoretical chemistry and experience with state of the art molecular electronic structure codes eg. Gamess, Orca, Turbomole, Gaussian, Molcas, etc
- The ideal candidate is a motivated and talented problem solver (Geek).
  - When you don't understand (or forget about something), do you look for it in the internet or with your colleagues and go back on track in less than a coffee break? We are waiting for you.
  - Is that stopping you if your computer is not working as you want and the IT people are "unavailable"?
- Proficiency in Shell and Python. Experience with other programming languages will be positively evaluated.
  - Are you more comfortable writing on a terminal than clicking on a graphical interface? We want you!!
  - Are you one of those heroes who don't panic if needing to install Python libraries to run more powerful scripts? Then, we will respect you as you deserve.
  - Have you written some handy scripts that you manage to use on most computers you work with? Then, we want to meet you!
  - Do you code a script if you need to do the same task more than 3 times on the same day? We can be friends!!
  - Do you prefer using your code (or open code) for plotting and analyzing numerical data to boring spreadsheet-based software? Here's your home!
  - You need some data for its usage as input in some other software/program, but it is not in the expected format. Is that something you can fix? Yes? Free coffee for you!
- Team player skills and enthusiasm to work in a multidisciplinary, collaborative environment

- Excellent command of the English language (fully fluent in writing and speech). No knowledge of German is totally fine (free lessons will be provided)

## **Offer**

We offer a deep immersion in modern materials designing for sustainable energy technologies; the candidate will learn and live the translational perspective of designing bio- and nano-hybrid materials for sustainable energy-related applications every day. The validation of the design will also be carried out in the chair by experimental members.

TUM offers a wide variety of inspiring and challenging Ph.D. programs, which will supplement the research training with outstanding opportunities for career development, continued education, and life-long learning.

Situated on the Bavarian forest gate, Straubing, the old ducal town on the Danube, is the intellectual hub for renewable raw materials and technologies for sustainability in Germany. Straubing, although small in the number of inhabitants, offers everything you need for a successful Ph.D., including a diverse selection of taverns, cafés, and beer gardens. TUM Campus Straubing for Biotechnology and Sustainability offers scientific and academic excellence in a student-friendly and fresh environment.

The successful applicant will hold a 3-year contract with the possibility to expand it up to 1 year. We offer a competitive salary and benefits depending on work experience and seniority in accordance with the public service wage agreement of the Free State of Bavaria - TV-L E13 (50-65%). As an equal opportunity and affirmative action employer, TUM explicitly encourages applications from women and all others who would bring additional diversity dimensions to the university's research and teaching strategies. Preference will be given to disabled candidates with essentially the same qualifications.

## **Application**

We are looking forward to receiving your comprehensive application including your letter of motivation (1 page), CV (including complete contact information for two references) and academic transcripts of records in English in a **single PDF file**, via email to [biofunmat@cs.tum.de](mailto:biofunmat@cs.tum.de) . **Please indicate only "PhD TM\_ML" in the subject line.**

The position will be open until the candidate is selected.

For further information, please contact:

Prof. Dr. Rubén D. Costa  
Chair of Biogenic Functional Materials,  
Technical University of Munich  
Email: [biofunmat@cs.tum.de](mailto:biofunmat@cs.tum.de)