The Cluster of Excellence *liv*MatS develops completely novel, bioinspired materials systems that adapt autonomously to various environments and harvest clean energy from their surroundings. The intention of these purely technical – yet in a behavioral sense quasi-living – materials systems is to meet the demands of humans with regard to pioneering environmental and energy technologies. The societal relevance of autonomous systems and their sustainability will thus play an important role in their development. The research program of *liv*MatS is characterized by highly interdisciplinary collaboration between researchers from a broad range of fields including engineering, chemistry, physics, biology, psychology, the humanities, and sustainability sciences.

The livMats Cluster of Excellence is offering the following position:
PhD position for Project **Chemistry of Triboelectric Materials**
(Envisaged start date: October 2022)

Project description
The triboelectric effect can be used to power functional materials systems by harvesting mechanical energy from their surroundings. Unfortunately, the underlying charge separation mechanisms are still elusive. This project aims to understand the basic charge separation processes and to identify molecules and materials with maximized energy harvesting efficiency. The triboelectric effect can be used to power functional materials systems by harvesting mechanical energy from their surroundings. Unfortunately, the underlying charge separation mechanisms are still elusive. This project aims to understand the basic charge separation processes and to identify molecules and materials with maximized energy harvesting efficiency.

In collaboration with excellent experimentalists you will solve one of the oldest outstanding problems in science and explain the origin of tribolelectricity. To do so, you will perform **density functional theory** (DFT) calculations to determine the extent and mechanism of charge transfer (electron, ion, material transfer) of the provided material pairs upon mechanical contacting. You will go beyond standard DFT and use constrained density functional theory (CDFT) in combination with Marcus theory to investigate the kinetics of charge transfer reactions especially in combination with mechanochemically induced molecule fragmentation and radical formation.

Candidate profile
You should have a M.Sc. degree in physics/chemistry or similar. A PhD thesis requires enthusiasm for scientific research, eagerness to learn new methods, high ability to work in a self-organized manner and willingness to collaborate in an international team. Experience with electronic structure calculations (especially DFT) and a strong related mathematical background are mandatory. Experience in scientific programing (Python, C++, Fortran) is highly advantageous.

Please hand in:

- Letter of intent detailing why you are interested in this specific project and how your previous research qualifies you for the project (up to 1,500 words)
- Curriculum Vitae with list of publications (if applicable)

- Certified copies of your university degree(s) with grades (BA and MA certificate / Diploma certificate and transcript)
- Short summary of your master's thesis (up to 1,000 words)
- Work sample (chapter from recent thesis or journal article, up to 5,000 words)
- Suggestion of two referees with contact details

Your documents will not be returned after the application process. For this reason, please submit copies only. This position is limited to 36 months. The salary will be determined in accordance with TV-L E13. We are particularly pleased to receive applications from women for the position advertised here.

Please send your application in English including supporting documents mentioned above citing the reference number by September 1st. Applications in written or electronic form are to be sent to the following address:

Contact person about position: Prof. Michael Moseler

Mailing address for applications:
Albert-Ludwigs-Universität Freiburg
Gregg Dubow
Freiburger Zentrum für interaktive Werkstoffe
und bioinspirierte Technologien (FIT)
Georges-Köhler-Allee 105
D-79110 Freiburg
Kennwort: livMatS

E-Mail address for applications: positions@livmats.uni-freiburg.de (please send one PDF file only)