

## Post-Doc Position at TU Darmstadt

The newly established LOEWE centre *Soft Control* investigates new functional surfaces whose properties can be switched by external stimuli such as light, electric or magnetic fields. This functionality is implemented by attaching polymers with switchable units to these surfaces.

Within the centre, our group simulates the expansion/collapse of photo-switchable polymers on a solid support. A typical system could consist of poly(ethylene oxide) brushes, which contain photoactive spiropyran units. Such a brush will be swollen in water when the spiropyran is in its zwitterionic form, and it will collapse when spiropyran is photoswitched into the neutral form. Resulting questions concern the mechanism of switching, the phase behavior of polymers of different composition for different spiropyran states, permeation and transport of different molecules through the polymer in different states of swelling, etc.

The work involves the use of advanced multi-scale molecular simulation approaches, which combine mainly atomistic and coarse-grained molecular dynamics (see references below), with some supporting quantum-chemical calculations. There is an intense cooperation between the research groups in *Soft Control*. Our theory project will have close interaction with several experimental groups who are involved in the preparation and/or characterization of photoswitchable surfaces.

For the project, we are looking for a **post-doctoral researcher** with a research background in theoretical chemistry, physics or materials science. The ideal candidate would have a solid knowledge (maybe a PhD) in a field like molecular simulation of soft materials, computational statistical mechanics, or theoretical polymer physics. Programming experience is essential, German-language skills would be an asset. Employment is initially for 1 year with the possibility of extension of up to 3 years. We aim to fill the position as soon as possible.

Please send your application to:

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### References:

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