Leibniz Universität Hannover

The Institute of Structural Analysis at the Leibniz University Hannover invites applications for the position of a

Research Associate/PhD Candidate (m/f/d) on the topic of "Reactive coarse-grained molecular dynamics simulations of nanoparticle/polymer nanocomposites" (Salary Scale 13 TV-L, 100 %)

to be filled by Dec 1st, 2022. The position is initially limited to 3 years, with the possibility of extension.

The topic
Synthetic nanocomposites are increasingly used in conditions where extreme mechanical loads have to be withstood. In the design of such materials, computer simulation techniques are becoming inevitable thanks to recent developments of modeling techniques and computational capacities. However, when it comes to predicting nanocomposite properties, current techniques fall short either of considering large enough systems (i.e. atomistic simulations) or accounting for the right underlying physics (i.e. continuum mechanics). In this ambitious project, we put forward a novel multiscale simulation protocol based on adapting and improving some existing techniques to develop coarse-grained models for nanoparticle reinforced polymer nanocomposites. The characterizing feature of this project is to derive reactive coarse-grained force fields using a mapping procedure from all-atom molecular dynamics simulations. It allows simulations of large atomistic systems with an accurate description of the breaking of chemical bonds to model damage mechanisms in the materials.

Tasks
The position offers an interesting research challenge at the interface of fundamental and applied research. The successful candidate will work on extending the state of the art regarding the molecular modeling and design of high-performance nanoparticle/epoxy nanocomposites.

Employment conditions
Formal requirements include a scientific university degree (master-level) in engineering, or related fields. The successful candidate will be provided with counsel and support, however, the ability for self-motivated and independent work is essential. This task requires a profound background in molecular simulations, computational mechanics and mechanics of materials. Knowledge concerning technological aspects of composites and practical engineering skills are beneficial. Willingness to support teaching activities is expected. Good English and basic German language skills are required.

The salary for the position is according to salary scale 13 TV-L, further information can be found online.

Leibniz University Hannover considers itself a family-friendly university and therefore promotes a balance between work and family responsibilities. Part-time employment can be arranged on request, as long as the offered workplace is covered in full extent.

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The university aims to promote equality between women and men. For this purpose, the university strives to reduce under-representation in areas where a certain gender is under-represented. Women are under-represented in the salary scale of the advertised position. Therefore, qualified women are encouraged to apply. Moreover, we welcome applications from qualified men. Preference will be given to equally-qualified applicants with disabilities.

Further inquiries may be directed to Prof. Dr.-Ing. habil. R. Rolfes (Email: r.rolfes@isd.uni-hannover.de) and Dr.-Ing. Sven Scheffler (Email: s.scheffler@isd.uni-hannover.de). Further information can be found on our website at: https://www.isd.uni-hannover.de/en/

Applications should include a curriculum vitae and the usual transcripts and certificates. All documents should be merged into a single PDF-file. Application documents should substantiate the applicants skills regarding the aforementioned aspects.

Please submit applications including above-mentioned documents by October 24th, 2022 with reference to the internal code **'position 124'** in electronic form to

Email: sekretariat@isd.uni-hannover.de

or alternatively via postal mail to:
Gottfried Wilhelm Leibniz Universität Hannover
Institut für Statik und Dynamik
Appelstr. 9A
30167 Hannover
http://www.uni-hannover.de/jobs

Information on the collection of personal data according to article 13 GDPR can be found at https://www.uni-hannover.de/en/datenschutzhinweis-bewerbungen/.