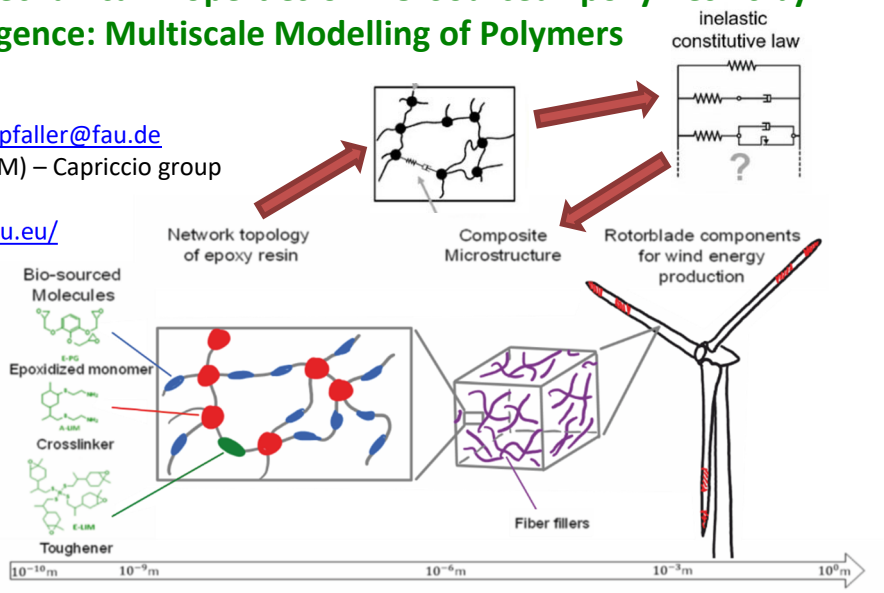
Doctoral Researcher Position

BIO ART: Optimization of Mechanical Properties of BIO-Sourced Epoxy Resins by ARTificial Intelligence: Multiscale Modelling of Polymers



Contact

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Start and End Date

Start Date: October 2023
End Date: September 2026

Scientific Areas

Mechanical Engineering, Mechanics, Materials Science, Chemistry, and related fields

Your Profile

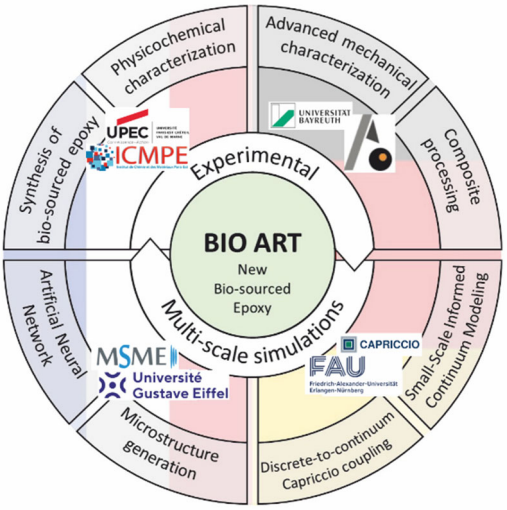
You are an excellent holder of a master degree in Mechanical Engineering, Mechanics, Materials Science, Computational Engineering, Mathematics, or related fields or expect to finish your master studies by September 2023 the latest. You have profound mechanical background together with knowledge in Continuum Mechanics, Finite Element method, and/or particle-based simulation techniques like Molecular Dynamics as well as programming skills in Matlab, C++, and/or Fortran90. You are highly interested in ***understanding fundamental principles of epoxy materials across the scales and disciplines*** as well as in ***linking experimental findings with numerical predictions***. Beyond this, you are eager to ***learn and develop new methods*** and want to work in an ***interdisciplinary and international environment***. You are open for short and/or medium term research stays (France and/or Germany) at the institutes involved.

Project Context and Environment

The present doctoral research project is part of the Franco-German research project “BIO ART” with partners from

- the Institut de Chimie et des Matériaux Paris-Est (ICMPE) at the Université Paris-Est Créteil Val de Marne (UPEC),
- the Laboratoire Modélisation et Simulation Multi-Échelle (MSME) at the Université Gustave Eiffel (UGE),
- the Department of Polymer Engineering (PE) at the University of Bayreuth (UBT), and
- the Capriccio group at the Institute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU).

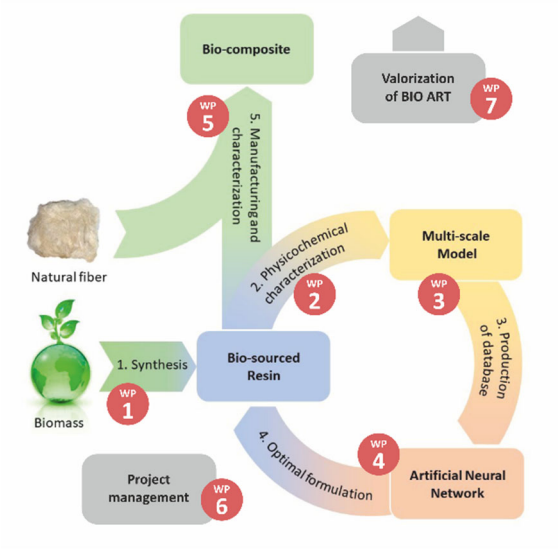
BIO ART’s main goal is to develop a fully bio-based epoxy-fibre composite at a competitive price with thermal and mechanical properties comparable or even superior to classical petro-sourced epoxy composites. In addition, BIO ART aims at proving the composite’s applicability on a semi-industrial scale by manufacturing demonstrators that address the typical geometrical and processing requirements of wind energy rotor blades as a model for further industrial applications. To this end, ***BIO ART integrates cutting-edge techniques of polymer synthesis, experimental characterisation, and simulations*** in an international framework.



Project Objectives

The doctoral research project offered here will be located at the Institute of Applied Mechanics (LTM) at FAU Erlangen-Nürnberg, whereby short and/or medium term research stays in Paris (ICMPE at UPEC, MSME at UGE) and/or Bayreuth (PE at UBT) are highly encouraged. The present project will start in October 2023 as a scientific continuation of a master thesis project

also hosted at LTM (please consider the associated call for positions), which studies the viscoelastic properties and the resin topology in order to choose and calibrate an appropriate continuum mechanical constitutive law. This preceding work will form the first step towards a structure-property relationship for the bio-based epoxy formulations to be synthesised and experimentally investigated at ICMPE.



BIO ART consists of five scientific work packages (WPs) and two WPs mainly comprising administrational and dissemination activities. ***The present doctoral project is mainly associated with WP3 "Multiscale Modelling"***, but will have close interactions with the remaining WPs. In particular, it leads the continuum mechanical investigations in

- ***WP3.bii "Viscoelastic properties of the continuum"***, which develops and calibrates a continuum mechanical constitutive law that establishes a link between the network structure of the epoxy formulations and their mechanical properties at larger scales and
- ***WP3.cii "Multiscale simulations of fracture"***, which develops a multiscale simulation tool that couples a fine-scale network model capable of polymer fracture at the network level with the coarse-scale continuum model providing realistic boundary conditions.

In both work packages, the present doctoral project will closely collaborate with MSME at Champs-sur-Marne near Paris, which is responsible for ***WP3.a***, ***WP3.bi***, and ***WP3.ci*** (see below). It will apply and further enhance multiscale techniques developed and employed within the Capriccio group (https://www.capriccio.research.fau.eu/) at LTM. In summary, ***WP3.bii*** and ***WP3.cii*** are closely interlinked with BIO ART's adjacent work packages:

- ***WP1 "Synthesis of bio-sourced epoxy"***, which is carried out at ICMPE, synthesizes neat bio-based resins, tougheners, and the resulting toughened resin formulations.
- ***WP2 "Characterisation of bio-sourced epoxy"***, which is a joint work package of ICMPE and the Department of Polymer Engineering, experimentally investigates the viscoelastic properties of the bio-resins synthesised in WP1 and their resin topology. To this end, highly demanding experimental studies using also nuclear magnetic resonance spectroscopy (NMR) will be performed to obtain insight into the polymer topology at molecular scale. Further advanced mechanical testing comprising fracture experiments with crack path tracking, crack front analysis, and fracture surface analysis will complete WP3 and provide experimental evidence for the modelling and numerical investigations focused in the proposed doctoral project.
- ***WP3.a "Generation of polymer network topology"*** together with ***WP3.bi "Viscoelastic properties of the MNMS model"***, both within the responsibility of MSME, will generate a "Macromolecular Network at Meso-Scale" (MNMS) model using particle-based simulations (molecular dynamics and Monte-Carlo), whose material specifications follow from the experimental findings in WP2. ***WP3.ci "Fracture phenomena at MNMS level"***, also lead by MSME, will introduce debonding phenomena at the atomistic level into the MNMS model and will thus make it capable of fracture simulations at the mesoscale. This, in turn, forms the basis for the multiscale simulation tool to be developed in the present doctoral project (cf. ***WP3.bii*** and ***WP3.cii***).
- ***WP4 "Optimization of bio-sourced epoxy formulation by artificial neural network"***, which is within the responsibility of MSME, will develop an artificial neural network framework to predict efficiently the mechanical properties of the toughened epoxy resin formulations to be synthesised and characterised in ***WP1*** and ***WP2***.
- ***WP5 "Composite processing and mechanical characterisation"*** led by the Department of Polymer Engineering provides an important step to industrial valorisation of BIO ART's bio-based epoxy formulations: It will manufacture bio-based epoxy composites at a semi-industrial scale and thus provide elementary insights into the processability and the material properties of the novel materials.

Our Offer

We offer an innovative and diverse research environment in an interdisciplinary team, great freedom for independent research activities, and a close exchange with international researchers in different disciplines. The position is a full-time position in salary group TV-L E13 (depending on your qualification) and limited to 3 years.
The FAU promotes professional equality for women. Women are therefore expressly encouraged to apply. Severely disabled persons within the meaning of the Severely Disabled Persons Act (Schwerbehindertengesetz) are given preferential consideration if they have the same professional qualifications and personal suitability.

Your Application

Please send your application (including cover letter, curriculum vitae, transcript of records and relevant documents) via email to sebastian.pfaller@fau.de. Applications will be accepted by February 28th, 2023 the latest. Selected applicants will pass an interview conducted in German or English. Incomplete applications will not be considered.