Kiel University
Christian-Albrechts-Universität zu Kiel

At the **Faculty of Engineering, Kiel University**, **Institute for Materials Science**, the **Chair for Bioinspired Materials and Biosensor Technologies** invites applications for the position of

Postdoctoral Research Scientist in Computational Materials Design, Molecular Modeling and Machine Learning

starting at the earliest possible date.

The position is initially offered for a period of three years. The regular weekly working time corresponds to that of a full-time employee. The salary is according to the German public sector collective agreement (TV-L E13). The position includes teaching responsibilities (teaching may be conducted in English) and offers the opportunity to pursue a habilitation.

We are an interdisciplinary and international research group with longstanding expertise in bioinspired materials and biosensor technologies. Our team comprises electrical engineers, chemists, chemical engineers, computational scientists, materials scientists, biomedical engineers, food scientists, and biotechnologists.

Our computational research integrates molecular mechanics (MM), molecular dynamics (MD), quantum mechanical (QM/DFT) calculations, molecular modeling, and machine learning to design next-generation bioinspired materials, synthetic receptors, molecularly imprinted polymers, nanocomposites, and functional interfaces. We develop computational methodologies and in-house machine-learning algorithms for receptor and materials design, with all computational predictions being closely integrated with experimental validation.

Responsibilities

1. Computational design of synthetic receptors and bioinspired materials
2. Molecular modeling of biomolecular recognition processes
3. Molecular dynamics simulations of proteins, peptides, polymers and interfaces
4. QM/DFT calculations for functional material characterization
5. Development of computational workflows integrating MM, MD, QM and machine learning
6. Design and optimization of molecularly imprinted polymers and nanocomposite materials
7. Development of AI/ML approaches for receptor and materials discovery
8. Collaboration with experimental researchers for computational-guided materials development
9. Scientific publications and presentation of research results
10. Participation in proposal writing and supervision of students
11. Teaching in computational (bio)chemistry, computational (bio)materials science or molecular modeling

Eligibility criteria

1. PhD in Computational Chemistry, Computational Biology, Bioinformatics, Computational Materials Science, or a closely related field.
2. Demonstrated experience in several of the following areas:
    a. Molecular mechanics (MM), molecular dynamics (MD), and quantum mechanical (QM/DFT) calculations
    b. Molecular modeling and molecular docking
    c. Enhanced sampling methods and free-energy calculations
    d. Machine learning and/or deep learning for molecular or materials design
    e. AI-assisted molecular and materials design
    f. Data-driven materials discovery

   g. Scientific programming (Python required; experience with other programming languages is an advantage)
   h. High-performance computing (HPC) and computational workflow development
3. Experience with widely used molecular simulation software (e.g., GROMACS, AMBER, CHARMM, NAMD, OpenMM, or equivalent) is desirable.
4. Strong interest in interdisciplinary and collaborative research.
5. Excellent communication, interpersonal, and organizational skills.
6. Excellent written and spoken English.
7. Strong scientific publication record and the ability to communicate research findings effectively through publications, project meetings, conferences, and seminar

We offer

1. Opportunity to contribute to multiple interdisciplinary research projects.
2. Salary according to TV-L E13, along with the social benefits provided by the German public sector (e.g., health insurance and pension scheme).
3. Opportunity to develop your own research project while working in a collaborative, team-oriented research environment.
4. An interdisciplinary, international, and supportive working environment.
5. Opportunities for collaboration with renowned research groups in materials science, electrical engineering, computer science, and medicine.
6. Access to state-of-the-art high-performance computing facilities and a modern supercomputing center.
7. Opportunity to conduct cutting-edge research at the interface of academia and industry.
8. Opportunity to gain teaching experience in an international academic environment.

Application deadline: October 31, 2026

How to apply

Please submit your application via the link below:

https://jobs.uni-kiel.de/jobposting/76f612f4746f60e09bf6b7d67ca721f0edee63dd0

For questions regarding the position, please contact Prof. Altintas's secretary at abu@tf.uni-kiel.de

Prof. Dr. Zeynep Altintas
Christian-Albrechts-Universität zu Kiel
Technische Fakultät
Institut für Materialwissenschaft
Bioinspired Materials and Biosensor Technologies
Kaiserstr. 2
24143 Kiel