



# Computational-Research-Scientist

**APPLY NOW**

## Context

Our flagship product [GRACE](#) has been developed with and for our customers for over twenty years. From the early days up until today, we have been tightly connected to the experimental departments of large pharmaceutical companies, embracing their problems as ours.

We have pioneered and become the world-leader of [organic Crystal Structure Prediction](#). With our pharmaceutical industry customers and staff from all around the world, we are inventing the next generation of [software tools for in silico materials design](#).

We rapidly deploy new technology to leading pharmaceutical companies. We put the principles of sustainable development into practice and offer an industrial working environment with an academic touch.

Our offices are located in [Freiburg](#) (Merzhausen), Germany, on the border of the [Black Forest](#). The city has a rich student life with a variety of places to unwind after work. The residential areas offer [green](#), calm surroundings that are ideal for healthy lifestyles and families. Close to France and Switzerland, the Black Forest is one of Germany's most touristic regions known for the beauty of its lakes and landscapes. In the wintertime the region offers good opportunities for alpine and cross-country skiing.

## Your responsibilities

As Computational Research Scientist you become one of the few world-leading experts in Crystal Structure Prediction and help our customers to make the most out of our software, [GRACE](#). When approached by pharmaceutical companies, you often are the last hope to solve hot or cold cases. You solve [solid-state mysteries](#) where experiments fail or are ambiguous, but calculations can lead the way.

You start in the next three months of the current year in a permanent position. You join a team of three experienced [Contract Research](#) Scientists and report to Dr. Marcus Neumann, the Science and IT Director and to Elsa Gheziel MA, the HR and Administration Director.

### **Contract research**

- Solve non standard solid-state problems in pharmaceutical development
- Compile scientific reports
- Assist customers with the interpretation of results
- Schedule and monitor computational tasks in an HPC environment
- Write scripts for data analysis in Python

### **User training and support**

- Answer users' questions by phone and email
- Write GRACE tutorials and documentation
- Design and deliver on-site user training

### **Research**

- Become an expert in using AMS' technology up to the point where you can publish high quality research and give oral presentations
- Explore industrial applications of CSP in close collaboration with customers and AMS' scientific software developers
- Identify scientific software development opportunities

### **Marketing**

- Represent AMS at conferences and commercial exhibitions
- Develop a scientific and industrial network
- Provide input for marketing material
- Support recruitment campaigns

# Your profile

## Soft skills: do you share our vision and values?

- Sharp and rational thinking combined with a pragmatic attitude
- Scientific ambition: you want to get the best results and lead the way
- Ability to act in the interest of the company: loyalty and dedication
- Ability to adapt your communication style on technical and scientific topics to non-experts, customers and members of AMS Team
- Soft human interface: cooperative, friendly manners in the in day-to-day interactions with colleagues and customers are a must
- Intercultural awareness and open personality are a must
- Commitment to Sustainability and Business Ethics are a must

## Hard skills: do you bring in...?

- Excellent written and spoken English
- Strong molecular modelling background
- Genuine interest for molecular crystallography, and willingness to learn
- Familiarity with experimental methods for solid-state characterization of organic materials
- Hands-on experience with at least 2 of the following:
  - Force fields and ab initio methods
  - HPC Linux clusters
  - Programming in Python
  - Rietveld Refinement or SDPD

## Education

PhD in solid-state physics, solid-state chemistry or crystallography, or a related science.

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# What we offer: a workplace to shape your future

We are a small family business with short communication paths. The impact of your work is immediately visible and directly supports other team members.

We aim to provide a professional environment in which people from all over the world at different stages of their lives can find the work-life balance that suits them.

Because we care about our employees, our customers' needs, scientific progress and the planet, working at AMS does have a meaning.

- Flexible work time management around core hours
- Free organic coffee & teas, fresh fruits
- Resilient, organic garden with a planter where employees can grow their own fruits and vegetables
- A quiet workplace with the quality of a living space (not open plan offices)
- Part-time work for some of the positions
- Job specific training
- Yearly: 28 days paid leave (full time based) + about 10 days public holidays
- Equal opportunity policy
- Help with settling in if you are located outside Germany

## What about recruitment at Avant-garde Materials Simulation?

Avant-garde Materials Simulation Deutschland is an [equal opportunities](#) recruiter: your application is welcome regardless of your age, gender, ethnic origin, disabilities or religion/beliefs.

What matters most to us, beyond your skills and experience, is your mindset. Tell us more about your philosophy at work and your soft skills in your application form under Your Motivation-s.

### Step 1

Fill-in [Application Form](#), and you get notified in case of successful completion.

### Step 2

Pre-screening of candidates by AMS Human Resources,

### Step 3

You are invited to take some hard and soft-skills tests,

and you get notified about early rejection, or Step 3.

and you get notified about rejection, or Step 4.

#### Step 4

Remote interview, and you get notified about rejection, or Step 5.

#### Step 5

On-site day in Freiburg: series of hands-on tests and interviews with AMS Management and the concerned Department.

#### Step 6

Decision on job offer, you get notified within 2 weeks.

## Curious?

### Visit our Website

Discover Avant-garde Materials Simulation Deutschland GmbH.  
Sharing common values is the basis for a diverse and happy Team!



### Our mindset

- We are addicted to innovation
- Our software is used by many large pharmaceutical companies
- Our customer's problems are our problems
- We are a family business
- We do business to invest in science, not the other way around

### Our Business Ethics

- Sustainable development
- Renewable energies
- Soft mobility and CO2 offset for travels
- Low energy consumption

- A culture of respect and openness towards colleagues and partners