The Research Center Pharmaceutical Engineering GmbH (RCPE) is a global leader in pharmaceutical engineering sciences. We help our partners create and manufacture advanced medicines for patients worldwide through optimizing products and processes.

For our team / Area 1 "Science of Quality" we are looking for an active, highly qualified (m/f/x)

SCIENTIST (with possibility to do a PhD)
Molecular Modeling - Chemistry
PhD possible
Ref. No 125

Duties and Responsibilities

- Apply state-of-the-art molecular simulation techniques, both classical and ab-initio/DFT based approaches, to establish properties and understand/predict the behavior of materials in pharmaceutical production processes (e.g., for prediction of mechanical properties, cohesion energy density, morphology/habits, or molecular mobility and disorder/amorphization propensities of API crystals.
- Develop new scientific ideas, methods, algorithms, and technologies.
- Actively participate in project teams/ meetings/ scientific networks.
- Report and present scientific/ technical results and contribute to publications & presentations.

Requirements

- An MS degree in theoretical chemistry, (bio-)physics, material science, or a related field.
- Hands on experience with classical molecular mechanics/dynamics and/or ab-initio/DFT simulation tools and methods, including a good understanding of the involved algorithms and theory.
- Experience in programming, (e.g., python, or C++) and familiarity with Unix/Linux systems, including common command line tools.
- Professional conduct and communication skills in dealing with international clients, partners and colleagues
- Interest in and experience with performing top-level and target-oriented research at the interface of basic science and industrial application.

Good to Have

- A good background in pharmaceutical manufacturing processes.
- Experience in the experimental characterization of materials.
- Experience with advanced simulation methodologies (e.g., extended ensemble techniques, use of ML-based potentials, or optimization of classical empirical force fields)
- Experience with common AI/ML libraries and tools.
- Familiarity with alternative algorithms and tools, such as population balance equation solvers, CFD, or DEM applications.

We offer

- A multidisciplinary and dynamic research environment and access to highly modern infrastructure on campus of Graz University of Technology
- Opportunities for career development at the academic and industrial level
- A competitive salary (min. € 42.000, - gross/year, overpayment - depending on qualification - possible).
- Possibility to work part-time

We are looking forward to receiving your application, indicating the ref. no., and including a cover letter, your CV, publication record and credentials.

Contact
https://careers.rcpe.at/