



The **Max-Planck-Institut für Kohlenforschung in Mülheim an der Ruhr**, founded in 1912, conducts basic chemical research aimed at making chemical transformations as energy and resource efficient as possible and catalysis with all its facets is at the center of the research.

The Department of Molecular Theory and Spectroscopy is presently looking for a

**Ph.D. student or post-doc researcher (f/m/d)
with expertise in theoretical chemistry**

and interest in development and application of embedding methods for simulations in complex environments. The position is financed by the *e-conversion* DFG cluster of excellence and will be based in the [Molecular Theory and Spectroscopy department](#) lead by Frank Neese.

Job description: Our new team member will focus on the implementation of efficient coupling terms in QM/MM embedding and applying our state-of-the-art spectroscopy methods for complex systems like active sites in solid catalysts. The platform of our developments is the ORCA package which is currently one of the world's most versatile and frequently used quantum chemistry packages. Communication of research results in journal articles and by oral presentations is expected as well.

Qualification: The ideal candidate should have

- a master or a Ph.D. degree obtained in Chemistry, Physics or related fields
- profound knowledge of electronic structure theory
- programming skills and experience in developing quantum chemistry codes
- excellent English language and communication skills
- a proactive mindset and goal-oriented work ethic

Job offer:

- for Ph.D students, part time (26 hours) research position (TVöD E13) limited to 3 years; for postdocs, full time (39 hours) position limited to 2 years
- exciting and challenging research project in one of the world's most recognized research facilities
- excellent and well-maintained infrastructure and administrative support
- involvement in interdisciplinary research projects in the field of catalysis

Applications:

Please send your cover letter, curriculum vitae, and a list of two references with names and contact information in electronic form to Prof. Dr. Frank Neese (neese@kofo.mpg.de), Max-Planck-Institut für Kohlenforschung, Kaiser-Wilhelm-Platz 1, 45470 Mülheim.

Closing date: October 20, 2021

The Max Planck Society strives to ensure a workplace that embraces diversity and provides equal opportunities irrespective of gender, nationality or disabilities of the applicants. The Max-Planck-Institut is signatory of the Charta der Vielfalt. More information on support for working parents and on our data protection policy can be found on our homepage: <http://www.kofo.mpg.de/en/career>