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We have vacancy for the following position to join our team:

# Research Scientist Computational Chemistry

# (Reference No. RES000985)

**GBU/Function:** R&I

**Direct Hierarchy (Position):** E2P2L Modeling Platform Leader

**Job family:** R&I

**Job Location:** Shanghai

**Country :** China

**No. of Needs:** 1

**Validate From :** October 24, 2018

**Contact:** raphael.wischert@solvay.com

## Vacancy description

For our Research & Innovation center in Shanghai, we are looking for a *Research Scientist Computational Chemistry* to investigate chemical and physical properties of materials, such as chemical processes occurring at solid / liquid / gas interfaces, adsorption phenomena on porous and non-porous materials, reactivity of polymers, high-throughput modeling of organic reactions, and (catalytic) reaction mechanisms. The successful candidate will work in a multidisciplinary and multicultural team dedicated to the development of eco-efficient products and processes, in collaboration with internal teams and external research institutions.

## Key missions

- Work in the Research and Innovation Center Shanghai for Solvay/CNRS Joint Lab – Eco-Efficient Products and Processes Laboratory (E2P2L), UMI 3464.
- Plan, perform, analyze and document calculations for the study of chemical reactivity and interfaces, also in collaboration with internal and external partners.
- Build project files with the most up to date literature and ensure the updates of such files during the lifetime of the projects.
- Supervise the work of interns and coordinate collaborations with external research institutions.
- Identify and promote the added value of modeling for R&D projects and propose corresponding modeling approaches, using his / her quantum and physical chemistry skills.

## Profile

- Doctorate or postdoctorate in computational chemistry, physics, materials science or a related discipline.
- Strong track record in applying quantum-chemical (DFT or wavefunction-based) and force-field based methods to the study of chemical reactivity, adsorption phenomena, and related properties.
- Experience with one or more additional techniques, such as machine learning, QSPR approaches, modeling of electrochemical phenomena, solvents effects, modeling of kinetics and thermodynamics.
- Knowledge of scripting languages (Python, Perl, bash …) is not mandatory, but considered a plus.
- Critical thinking and strongly problem-oriented work style.
- Good ability to work in a team and communicate with internal and external stakeholders.