HUMBOLDT-UNIVERSITÄT ZU BERLIN
Mathematisch-Naturwissenschaftliche Fakultät I
Institut für Chemie

In the Quantum Chemistry Group (Professor Sauer) at Humboldt University, Institute of Chemistry, (http://www.chemie.hu-berlin.de/forschung/quantenchemie)

two post-doctoral positions for computational chemists/physicists (01.10.2012 – 30.09.2015)

are available in the following areas

Ab initio computer simulation of large chemical systems (AN/094/12)

with applications predominantly in heterogeneous catalysis (UNICAT cluster of excellence: http://www.unicat.tu-berlin.de/Research.24.0.html) and adsorption of small molecules (relevant for energy research) in metal-organic frameworks and zeolites.

Candidates are expected to have a PhD in Theoretical Chemistry/Physics and experience in non-routine applications of simulation codes to complex systems, including periodic boundary conditions. Profound knowledge of different methods for potential energy calculations (QM, QM/QM, QM/MM, force fields) is also required.

Quantum chemical methods for large chemical systems (AN/095/12)

With applications to molecule-surface interactions and heterogeneous catalysis (UNICAT cluster of excellence: http://www.unicat.tu-berlin.de/Research.24.0.html). Depending on the preferences of the applicant, this may include the further development or implementation of techniques and algorithms for accurate calculations of potential energy surfaces or the quantum solution of nuclear motion equations for anharmonic potentials.

Candidates are expected to have a PhD in Theoretical Chemistry/Physics and profound knowledge of quantum chemical methods, including wave-function-based electron correlation methods, and/or quantum methods for nuclear motions in anharmonic potentials.

Applications of qualified female scientists are encouraged.

Applications should mention the codes AN/094/12 and AN/095/12, respectively, and should be sent, preferentially in electronic form, as soon as possible (closing date October 1st) to:

js@chemie.hu-berlin.de
Humboldt-Universität zu Berlin, Mathematisch-Naturwissenschaftliche Fakultät I, Institut für Chemie, Prof. Dr. Sauer (Sitz: Brook-Taylor-Str. 2) Unter den Linden 6, 10099 Berlin.