



**UNIVERSITÄT
HEIDELBERG**
ZUKUNFT
SEIT 1386

Postdoctoral Position in Theoretical Chemistry (2 yrs.)

Our group offers a postdoctoral position in Theoretical Chemistry with a clear emphasis on relativistic quantum chemistry in theory and implementation. The main research topic focuses on the calculation of excitation/emission spectra for medium-sized organic complexes of Ir and Pt in order to model organic light emitting diodes (**OLEDs**). Hereby relativistic propagator and coupled-cluster methods as available in the **DIRAC** program package play a central role. Incorporation of solvent effects into the propagator method will be one of the major tasks in addition to developing protocols for the analysis of ligand effects on the emission spectrum. Furthermore, the feasibility of a multireference initial wave function for a polarization propagator shall be theoretically investigated since single-reference descriptions of transition metal compounds are often insufficient.

It is required that a possible candidate provides good background in relativistic quantum chemistry and possesses advanced skills in programming (Fortran90, C, MPI parallelization, scripting).

For further information please contact:

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