



MAX-PLANCK-INSTITUT
FÜR CHEMISCHE PHYSIK FESTER STOFFE

Ph. D. proposal – Materials Science



Scientific context

Replacing noble metals by low-cost substitutes is a great challenge in heterogeneous catalysis. Heterogeneous catalysis on complex intermetallic compounds, e.g. intermetallic compounds with large unit cells, represents a quickly growing field, which contributed to innovative breakthroughs in recent years.

The design of stable, active and selective intermetallic catalysts requires a multi-technique approach, based on ab initio calculations combined with experimental measurements :

- Understanding the chemical bonding in bulk complex intermetallic compounds helps to identify driving forces for the surface stability and rationalize the molecule/surface interactions and catalytic properties. It will be addressed at Max Planck Institut für Chemische Physik Fester Stoffe (MPI CPfS) in Dresden, Germany, using a combination of experimental (bulk diffraction) and quantum chemical calculations.

- The knowledge of surface structures is crucial to the understanding of catalysis processes. Surfaces will be investigated at Jean Lamour Institute (IJL Nancy, France), by a combination of surface science techniques and calculations based on Density Functional Theory.

Research group The research will be performed at Max Planck Institut für Chemische Physik Fester Stoffe (Dresden, Germany, main part) with long stays at Jean Lamour Institute (Nancy, France). The research will be supervised by Prof. Y. Grin (MPI CPfS, Dresden, Germany) in collaboration with Prof. É. Gaudry, Dr. V. Fournée and Dr. J. Ledieu from IJL Nancy (France).

Eligible candidate We are looking for a motivated student holding a master degree in materials science and/or solid state chemistry/physics.

Application instructions Send a resume, statement of motivation, grades for the past two years and email of two contacts to É. Gaudry, V. Fournée and J. Ledieu

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