## **Post-doctoral position**

Molecular spintronics: conductance and spin torque in molecular devices from first principles

#### **Supervisor:** Dr. Richard Korytár, http://korytar.eu.pn **Location:** Charles University in Prague, Czech Republic

## Description

The purpose of the project will be to investigate the interaction of an electric current with magnetic impurities in molecular junctions and molecular films (graphene ribbons, for example) with sizable spin-orbit coupling. The notion of molecular spin-torque is of particular interest here.

The consequences of quantum interference (two and multiple impurity scattering) will be examined with an eye on applications in (molecular) spintronics.

## Methodological framework

Density functional theory (ground-state properties and effective scattering states), nonequilibrium Green's functions (non-linear transport in presence of finite bias [1], current density [2] and spin torque [3])

## **Requirements**

The candidates must have a strong background in computational physics/chemistry or materials science. Some experience with programming, unix environments or high-performance computing is welcome. The project takes place in a high standing theoretical collaborative network. The one-year fellowship can be initiated immediately and extended until the end of 2019 conditionally. PhD must be obtained before the start of the contract.

# Gross monthly income: 45000,- CZK

The project will take place at the theory group, <u>http://theory.kfkl.cz</u>, Department of Condensed Matter Physics, Charles University in Prague. The research environment has a strong background in magnetism, quantum transport and electronic structure theory.

#### How to apply

A resume (with names of references) and a cover letter should be emailed to <u>korytar@karlov.mff.cuni.cz</u> Informal inquires are encouraged.

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#### References

 [1] A. Bagrets. Spin-polarized electron transport across metal-organic molecules: A density functional theory approach. J. Chem. Theory Comput., 9:2801, 2013
[2] M. Walz, J. Wilhelm, and F. Evers. Current patterns and orbital magnetism in mesoscopic DC transport. Phys. Rev. Lett., 113:136602, 2014
[3] F. Freimuth, S. Blügel, and Y. Mokrousov. Direct and inverse spin-orbit torques. Phys. Rev. B, 92:064415, 2015