

NEXT Invited Scientists

Guest name **KNECHT Stefan**
Position Independent Researcher
Affiliation ETH Zürich
Host laboratory in NEXT Laboratoire de Chimie et de Physique Quantiques – groupe SEM
NEXT contact (name and e-mail) Hélène Bolvin
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Dates of stay From January 9 to February 5, 2017

Brief Biodata

Born in Würzburg (Bavaria) in 1979.

Diploma in chemistry from the University of Heidelberg in 2005, Diploma thesis written in the group of Prof. L. Cederbaum, PhD ("*summa cum laude*") in theoretical chemistry from the University of Düsseldorf with Prof. Timo Fleig and Prof. Christel M. Marian in 2009. Nov. 2009 - Oct. 2010 postdoctoral research stay at the University of Strasbourg with Prof. Trond Saue, Nov. 2010 - Jan. 2013 postdoctoral research stay at the University of Southern Denmark in Odense with Prof. Hans Jørgen Aagaard Jensen. Since Feb. 2013 senior postdoctoral researcher with Prof. Markus Reiher at ETH Zürich.

Awards include a Marie Curie PhD research fellow ship (project NANOQUANT) from Jan. 2007 - March 2007 at the University of Southern Denmark in Odense with Prof. Hans Jørgen Aagaard Jensen and an individual postdoctoral grant (2 year fellowship) founded by the Danish research council for natural sciences in 2010.

Research project during the visit at NEXT

Descriptive Title Calculation of magnetic properties with the SO-DMRGPT2 method.
During his stay, Stefan Knecht has initiated the people of the LCPQ to the new method SO-DMRGPT2 : he taught about the fundamentals of the method and how to apply it on some specific molecules.

The SO-DMRGPT2 method has been recently developed in Zürich and permits to calculate the properties of open-shells molecules including spin-orbit and correlation effects using very large active spaces.