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IGNACIO FERNÁNDEZ GALVÁN

From Sweden to France

Project: **Electronic structure, conical intersections, and molecular dynamics**

Research topic: **Chemistry**

Swedish Institution: **Uppsala University**

French Institution: **CEISAM, Université de Nantes**

Dates of mobility: **07/03/2020** to **14/03/2020**

Program: **SFVE-A (ex FRÖ)**

PRESENTATION

Ignacio Fernández Galván is a researcher at the Department of Chemistry, Uppsala University. He studied and obtained a PhD degree in the University of Extremadura (Spain). His research there was focused on the development of the ASEP/MD method for studying solvent effects, with high-level quantum methods and an atomistic, statistically averaged representation of the solute. He spent two years in Grenoble (France), working on QM/MM calculations on proteins, with Prof. Martin Field. His interest then shifted to photophysical processes in solution, studying phenomena such as dual fluorescence. Since 2013, he contributes to the development of Molcas, a frontline quantum chemistry software package.

ACTIVITIES IN FRANCE

At Uppsala University, Ignacio Fernández Galván's research project dealt with the interaction between light and matter, more precisely chemiluminescence, which is the emission of light induced by a chemical reaction. The first step of chemiluminescence is chemiexcitation, which is the population of electronic excited states because of a chemical reaction. This transfer of population from the electronic ground state to electronic excited states occurs in the vicinity of the so-called conical intersections where the coupling between electrons and nuclei is strong. The topography of the conical intersections is known to determine the chemiexcitation yield. The aim of the stay in France was to pursue a collaboration with the Laboratory CEISAM, at Université de Nantes, to try to quantify the effect of the topography of the conical intersections on the efficiency of chemiexcitation.

Thus, Ignacio Fernández Galván visited Dr. Morgane Vacher, with whom he already worked in the past. They had the opportunity to plan future projects regarding electronic structure, conical intersections, and molecular dynamics.