

**ESR 2** Density Functional Theory calculations of the catalytic activity of PAHs and their interaction with grain surfaces

Host Institute: Institute for Physics and Astronomy, Aarhus University

Host Country: Denmark

Start date: During the period October 1<sup>st</sup> 2016 – September 1<sup>st</sup> 2017

The candidate will be employed at the Institute for Physics and Astronomy at Aarhus University and will be enrolled in the PhD programme at Aarhus University under the supervision of Prof B. Hammer.

### **Project description**

The rates of formation of small molecules like H<sub>2</sub>, OH, H<sub>2</sub>O and NH<sub>3</sub> in the interstellar medium can be greatly enhanced through catalytic effects. PAHs are proposed to act as catalysts for the formation of such species and this theoretical surface science project aims to elucidate these reactions. Specifically the aim is to: i) Calculate binding energies and addition barriers for oxygen and nitrogen on PAHs. ii) Calculate preferential adsorbate/functionalisation structures, iii) Calculate structural models for interstellar carbonaceous or silicate type nano-particulate dust grains, iv) Calculate the physisorption, chemisorption, and grafting of PAHs onto the surfaces of such dust grains, v) Calculate potential energy surfaces (PES) for Eley-Rideal type reactions, vi) Calculate pathways for conversion of small PAHs into larger PAHs/graphene layers. The project will include secondments to University of Milan (Italy) and Universite Paul Sabatier, Toulouse (France) for dynamic calculations for PAHs functionalization and reactivity and Graphic Science Ltd., our outreach-focussed enterprise partner, in developing outreach activities. The candidate will be enrolled in the Graduate School of Science and Technology at Aarhus University and will be expected to complete a PhD program which includes completion of local academic training requirements.

### **Group description**

The Theoretical Surface Science Group at Aarhus University carries out research in the field of density functional theory calculations in surface and nanoscience with a particular emphasis on automation of equilibrium structure and reaction pathway determinations. <http://phys.au.dk/forskning/forskningsomraader/condensed-matter-physics/theoretical-surface-science-group/>. The group has extensive experience in the development and application of density functional theory techniques and works closely with experimentalists.

### **Institute description**

The Graduate School of Science and Technology (GSST) is the largest graduate school at Aarhus University with almost 800 PhD students enrolled. PhD programmes at GSST are well structured, and participation in PhD courses, visits to international research institutions or universities and dissemination of knowledge are parts of the PhD education. Aarhus is Denmark's second largest city, a true student town, compact and close to the sea.

### **Ideal candidate**

The successful candidate will have a masters' degree (or equivalent) in physics, chemistry or astronomy. Programming experience is required and candidates with experience using UNIX/Linux operating systems and coding in python will be preferred.

**Working conditions and benefits**

The candidate will become an employee of the Dep. Phys and Astron. and receive a competitive monthly gross salary in accordance with the EC Marie Skłodowska-Curie. The contract period will last for 3 years.