

PhD position

Computational strategies for Raman characterization of complex nanomaterials

Supervisors: Prof. Frederik Tielens, Vrije Universiteit Brussel (VUB) Belgium

Prof. Monica Calatayud, Sorbonne Université (SU) France

Dates : september 2022 – august 2025 (3 years)

salary: ~2000 EUR/month

We look for a motivated candidate for a 3-year PhD in cotutelle between VUB and SU. The project is funded by the H2020 RIA project “*CHARISMA: Characterization of materials by harmonized Raman measurements*” and involves a pluridisciplinary collaboration between experimentalists, data scientists and physico-chemists in industry and academia. The target is to create a virtual centre of excellence on the characterisation of materials with Raman Spectroscopy for the advantage of the European Industry.

Keywords: DFT, Theoretical Chemistry, Raman Spectroscopy, materials characterization, materials development

Job description

The PhD project will be devoted to optimize and use strategies to simulate, analyze and compare Raman spectra for a set of complex nanosized materials. The computational approaches will involve quantum DFT-based calculations combined with molecular dynamics. Three families of materials will be studied: document nanomarkers based on inorganic crystals, plastic-based wrapping for food preservation and zeolite synthesis for catalytic applications. The candidate will design structural models to investigate the Raman response used in the applications cited above, and will use commercial codes (VASP, CRYSTAL, CP2K...) to optimize calculation protocols. The obtained modeling results will be compared with experimental results obtained by the CHARISMA partners, and will be used to guide, analyze and improve the industrial applications.

This position is open for applicants with a background in modelling with DFT and/or force field calculations in the field of theoretical chemistry, materials science, catalysis, and preferably with experience in periodic calculations. Besides a strong scientific background, it is important that the candidate has a good technical writing ability and verbal communication skills (English), and is willing to interact with the pluridisciplinary team of the CHARISMA project. The candidate shall spend mobility periods between Brussels and Paris of at least 1 year (can be split in shorter terms) in the frame of the cotutelle agreement. He/she will be doctor from VUB and SU. Students with high grades and research experience in their B.Sc. and M.Sc. studies in chemistry, physical chemistry or materials science from top universities are encouraged to apply.

Applications should be sent to frederik.tielens@vub.be and monica.calatayud@sorbonne-universite.fr with the subject: "Application for a Ph.D. CHARISMA PROJECT". The application should include a CV, a cover letter describing why the candidate should be considered for this position, transcripts of the B.Sc. and M.Sc. courses and grades, and a list of two professors/advisors that have supervised the student in his/her B.Sc. and/or M.Sc. research project and are willing to provide a letter of recommendation.