

Hosting offer for Marie Sklodowska-Curie Postdoctoral Fellowships (PF) 2022 at University of Antwerp/research group PLASMANT/Centre of Excellence NANOlab

<u>MSCA Postdoctoral Fellowships</u> are individual research grants offering excellent <u>postdoctoral</u> researchers the chance to develop their skills by means of international mobility. Through the implementation of an original and personalised research project, MSCA Postdoctoral Fellowships aim to foster excellence through training and mobility and to equip researchers with new skills and competences in order to identify solutions to current and future challenges.

University of Antwerp/research group PLASMANT invites motivated postdoctoral researchers to jointly prepare an application for the <u>MSCA-PF-2022 call</u> <u>Marie Skłodowska-Curie Postdoctoral Fellowships</u> call (<u>MSCA-PF-2022</u>) with them as host organisation.

Description of Hosting organisation/group

The PLASMANT research group has a wide expertise on atomic scale surface simulations as well as macroscale plasma simulations. The main research activities of the group are focused at developing and applying numerical models for gas discharge plasmas, the interaction between a plasma and a solid surface, and the interaction between a laser and a solid surface with the aim to optimize the applications of plasmas and lasers in materials science, nanotechnology, analytical chemistry, environmental and medical applications. For the interaction of plasmas and surfaces, classical molecular dynamics simulations are used, frequently combined with Monte Carlo simulations to study the dynamical evolution of the substrate, such as e.g. the morphology, structure, composition and physicochemical properties as a function of the interaction with the plasma. The PLASMANT group also develops reactive force fields for use in atomistic classical simulations.

For its computations, the PLASMANT group has access to the Flemish supercomputer Calcua at the UAntwerp. Moreover, PLASMANT has also built its own computer cluster. The group uses a host of codes, including home-written codes, as well as commercial software or software under academic licence, including ADF, BAND, VASP, ReaxFF, COMSOL and FLUENT.

Link to the webpage of the host group: <u>https://www.uantwerpen.be/en/research-groups/plasmant/</u>

Topics/expertise

Research interests in the group include the development and application of novel algorithms in the field of <u>atomistic simulations of nanomaterials</u>, with a chemically inspired setting. Simulating physical and chemical processes at surfaces of nanomaterials provides mechanistic information complementary to experimental data. The goal of the research in the group is to extend the applicability, range and scope of such simulations in both scale and complexity. Of particular current interest is directed growth of carbon nanotubes, plasma catalysis and novel nanomaterials.

Applications in the domain of <u>astrochemistry</u> are also welcome and should be focused around DFT (and classical) calculations for ice chemistry: how do molecules, relevant for the interstellar medium, interact with ice surfaces at 10 K, and how can chemical reactions proceed under such conditions? Topics of specific interest are the influence of charge, and the reaction mechanisms.

Supervisor interested in supporting the MSCA application: <u>Prof. Erik Neyts</u> (https://www.uantwerpen.be/en/staff/erik-neyts/)

Expertise: Computational techniques: * Atomic scale simulations * Molecular dynamics and Monte Carlo * Long time scale dynamics (hyperdynamics, metadynamics) * Density Functional Theory Materials and processes: * Plasma - surface interactions * Carbon nanotubes and graphene * Plasma catalysis * Nanoclusters * PECVD

Your profile

- Expected qualifications/expertise of the candidate: computational chemistry, materials science, with PhD degree in Chemistry or Physics
- You must have a completed PhD at the time of the call deadline (14 September 2022).
- Candidates must have a maximum of 8 years full-time research experience from the PhD award date until September 14, 2022. Periods of inactivity in research (e.g. unemployment, periods of employment outside research, parental or sick leave) do not count towards the time of research experience.
- For European fellowships, candidates can be of any nationality and must not have resided or carried out their main activity (work, studies, etc.) in Belgium for more than 12 months in the 36 months immediately before September 14, 2022.
- Highly motivated candidate with an excellent research track record appropriate to career stage, as evidenced by academic publications and other scientific output.

What we offer

- Support and guidance for the preparation of your MSCA PF proposal
- A stimulating, interdisciplinary environment for high-level research.

How to apply?

Indicate your interest by contacting the host institution as follows:

Please contact <u>lucian.covaci@uantwerpen.be</u> by e-mail with a short CV and motivation to indicate your interest to prepare a MSCA-PF application. Further details on research topics should be addressed directly to <u>erik.neyts@uantwerpen.be</u>.

After the supervisor agrees to support you as a MSCA-PF candidate, you can start preparation of MSCA PF project proposal and will be supported further by the supervisor and the Research Support Office of the host university.

For more information on the MSCA PF scheme or the host institution, you can contact the MSCA coordinator of the University of Antwerp: Dr. Liesbet Cockx (Research, Innovation & Valorisation Antwerp, Grants Office): <u>Liesbet.cockx@uantwerpen.be</u>.