NovaMechanics
Cheminformatics & Nanoinformatics Excellence

Ph.D. position in Computational Chemistry/Polymers Degradation funded by PlasticUnderground Marie Curie ITN

The PlasticUnderground Doctoral Network (DN) is an international, multi-partner, inter-sectoral doctoral research-training network with the aim to prepare an international cohort of Doctoral Candidates (DCs) in the development of solutions to the emerging plastic pollution crisis in soils and groundwater. Given the evolving understanding of subsurface soil and groundwater ecosystems as long-term storage pools of micro- and nanoplastics, interdisciplinary capacity that can support and provide guidance for the management of these systems, as well as development of adequate technological, social behavioural and legislative solutions is urgently needed. This interdisciplinary DN will integrate comprehensive training opportunities in cutting edge technological innovations, regulatory and behavioural approaches across traditional disciplinary and sectoral boundaries. The consortium comprises universities, research institutions and companies located in the UK, France, Spain, Serbia, Italy, Switzerland, Cyprus and Germany.

NovaMechanics (NovaM), an SME specializing in cheminformatics and nanoinformatics, is seeking for a Doctoral Candidate (DC) to join our team in Larnaca, Cyprus. The DC will work in the context of PlasticUnderground Marie Curie ITN, on developing new models for simulating the degradation of polymers under different soil systems and validating these models by comparing predictions with laboratory measurements. A key part of this study is understanding the effect of Manganese Peroxidase (MnP) on degradation, which will be studied at different scales. The PhD research, funded by the Marie Skłodowska-Curie Action (MSCA), will last for 36 months and require the DC to spend 8 months at the University of Birmingham (UoB) and 2 months at PolyMateria Limited (PolyM).The DC will employ a multiscale computational approach and have the chance to learn and use various computational methods, such as Density Functional Theory, Atomistic and Coarse-Grained Simulations, Monte Carlo Simulations, and Machine Learning Techniques.

DCs can be of any nationality but must comply with the following mobility rule: At the time of selection by NovaM (host organization), they must not have resided or carried out their main activity (work, studies, etc.) in the country of their host organization (Cyprus) for more than 12 months in the three years immediately prior to their recruitment. Candidates must demonstrate that their ability to understand and express themselves in both written and spoken **English** is sufficiently high for them to derive the full benefit from DN training. DCs must not yet be in possession of a doctoral degree at the date of recruitment.

Responsibilities

- Develop models for simulation of biodegradable MnP degradation under various soil systems.
- Simulate particle degradation and additive leaching.
- Quantification and prediction of future environmental residence times of new material based MnP and their size fractions in different types of environmental underground settings.

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- Driving and organizing collaborative efforts with internal and external partners

Desired Requirements

- Bachelor's degree in Chemistry, Chemical Engineering, Physics, Material Science, Environmental Science, Chem-Bioinformatics or other related Science.
- M.Sc. degree in Chemistry, Chemical Engineering, Physics, Material and Environmental Sciences, or other related Sciences. (Candidates holding a 5-year MEng degree are not obliged to have a MSc. Degree)
- Proficiency in English
- Strong programming skills (Python, Java, C++, Fortran, etc.)
- Diploma Thesis or Master Thesis in the field of Computational Chemistry or a related field will be appreciated (A web hyperlink of their Diploma or Master Thesis could be included in the attached CV)
- good knowledge of Linux operating system (i.e., writing bash scripts)
- knowledge of open-source computational software (i.e., OpenMM, LAMMPS, GROMACS, DLPOLY, NAMD, Quantum Espresso, CP2K, RASPA, Cassandra, OPENFOAM etc

What we offer

- An international work environment, in which you can develop your talent and realize ideas and innovations within a competent team
- Gross Salary (total cost with Cyprus coefficient): 2635€/per month. Mobility allowance 600€/per month (gross-total cost), family allowance if applicable 495€/per month (gross - total cost)
- An individual and well-structured training within the Marie Curie ITN network

How to apply

The candidate should submit a detailed CV and a cover letter matching the above according to his/her expertise. Two recommendation letters are needed from industrial or academic environments. The recommendation letters should not be general and should be referred to the above qualifications. Incomplete applications will be ignored.

All the above should be submitted until 30/09/2023 to hr@novamechanics.com with Ref: **MarieCurie2023Degradation**.