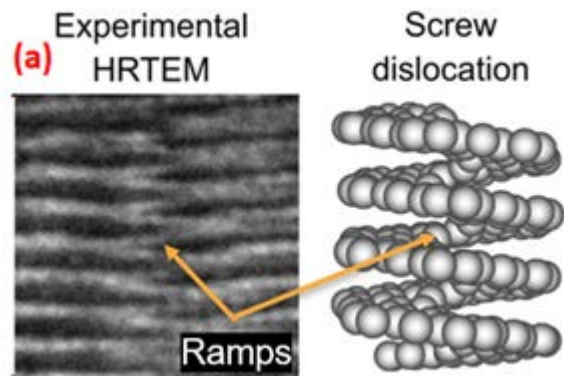## PhD Thesis Proposition

Dislocations in layered carbon nanomaterials

Institute of Materials Jean Rouxel (IMN), Nantes, France   www.cnrs-imn.fr

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Defects dominate the behaviour of layered materials such as graphite, BN and MoS_2, but research to date has focused on 0D point defects like vacancies; 1D dislocations have been largely overlooked, despite being common and observed in all layered materials[1]. Dislocation theory has been developed for 3D crystalline solids since the 1950s, and is responsible for key materials behaviour such as plastic deformation, mechanical strengthening, impurity migration and aggregation, optoelectronic processes, and crystal growth. Conventional theory does not take into account the anisotropy and new physics possible in 2D-layered materials. Dislocated layered materials are

fundamentally different compared to their non-dislocated equivalent. For example, screw dislocations turn a stack of separate layers into a continuous spiral surface, and dominate graphite formation processes.

The Project: This atomic-scale modelling PhD will explore the structure, formation and behaviour of screw and edge dislocations in layered materials, focussing initially on graphite, but extending to BN and other layered materials if time permits. We will explore their spectroscopic signatures, intercalation behaviour (critical for battery electrodes), and potential key role in superlubrication. We will use a range of modelling techniques such as density functional theory, xTB, and potentially machine learning approaches. The project will involve close collaboration with project partners in Lyon, Bordeaux, the UK, Spain and Australia, with the potential for experimental work in spectroscopic characterisation of relevant samples.

The Location: The PhD is at the Institute of Materials de Nantes Jean Rouxel (IMN), in the Physics of Materials and Nanostructures group. The IMN is one of France's primary materials research laboratories, run by the CNRS national research organisation at Nantes University. It has a strong international reputation in applied materials modelling and nanocarbon materials. Nantes is a lively and active city, on the edge of Brittany, western France (2h train from Paris)

Pre-requisites: A highly motivated candidate looking for a challenging PhD, with a good combination of scientific curiosity and imagination, coupled with scientific rigour. They will need to be flexible, interested to collaborate internationally, and at ease with both theoretical modelling and experimental spectroscopy. They will have a strong background in physics / physical chemistry / materials science (to Masters level), and a good level in spoken and written English. Experience with linux, python, ... is an advantage.

Practical Details: This PhD is funded by the CNRS through the ANR scheme for a duration of 36 months, salary is at the standard national rate (around 1770€/month before tax). The PhD will be conducted in English and/or French, but given the international collaborators a good level of English is required. Additional scientific and soft-skill training courses will be provided as part of the PhD.

Candidates should apply through the CNRS employment portal:

https://emploi.cnrs.fr/Offres/Doctorant/UMR6502-CHREWE-002/Default.aspx?lang=EN

with a covering letter detailing their interest in this specific post (generic applications will not be treated) and a CV. The position begins in October 2024 but with some flexibility on start date. Candidates will be pre-screened with some selected for remote interview. There is no restriction on candidate nationality but any candidate must pass governmental ZRR security pre-screening imposed at the laboratory.