Project Title: Synthesis and Characterisation of 2D-Material Heterostacks

Location: AMBER and School of Chemistry, Trinity College Dublin

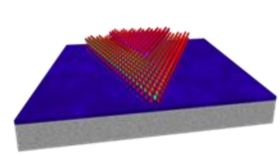
Supervisor: Niall McEvoy

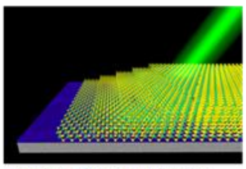
Start Date: October 2016, Duration: 4 years

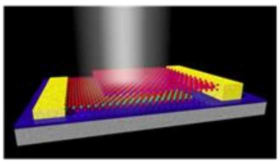
For further details contact nmcevoy@tcd.ie

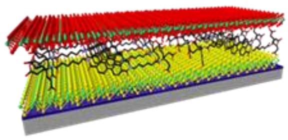
Applicant Criteria: A skilled, motivated and enthusiastic candidate is sought for a 4 year SFI-funded PhD project on the synthesis and characterisation of 2D-material heterostacks. Candidates must hold, or soon hold, a Master's or strong Bachelor's level degree in Chemistry, Physics, Materials Science or a related discipline. Applications will be considered from EU candidates only due to limitations on the funding available for fees. The project will primarily be conducted in the ASIN group labs in AMBER (Advanced Materials and BioEngineering Research Institute) and the studies will be undertaken through the School of Chemistry, Trinity College Dublin. While the project is associated with the School of Chemistry, it is interdisciplinary in nature and some background in any of physics, materials science and engineering, in addition to chemistry, would be beneficial. The project will be mostly experimental so previous lab experience is desirable. The ability to work both independently and as part of a team in addition to excellent oral and written communication skills will also be required for the successful realisation of the project.

Project Overview: This project will focus on the synthesis of 2D materials, particularly transition metal dichalcogenides (TMDs), and vertical heterostacks formed from them. Robust, vapour-phase synthesis routes will be developed with a view to integrating these materials into optoelectronic devices in a cost-effective and scalable manner. Novel characterisation pathways for these materials, including low-frequency scanning Raman spectroscopy and optoelectronic characterisation, will be developed in tandem with their synthesis. Additionally, a fundamental study on the effect of sandwiching molecules between these 2D layers will be undertaken. Thus the work encompassed fits primarily in oriented basic research but will also inform future applications-focused research.


CVD Synthesis of Heterostacks


Raman Characterisation


Optoelectronic Measurements


TMD-Molecule Sandwiches

2D materials have moved to the foreground of materials science research due to their exciting properties which mark them as promising candidates for prospective applications, particularly in electronics, optoelectronics and energy. While graphene is the most heavily studied of these materials to date, semiconducting 2D TMDs, such as MoS_2 and WSe_2, have attracted significant recent attention. Unlike graphene, these materials possess an appreciable bandgap, making them potentially useful as channel materials for assorted devices. 2D layers with different intrinsic characteristics (e.g. metallic, semiconducting, p-type, n-type etc.) can be synthesised and the combination of such layers, with complementary properties, affords exciting new possibilities in the construction and design of ultra-thin devices. Heterostacks, consisting of two or more 2D materials in vertical contact with each other, can preserve the unique properties of each monolayer material and, importantly for applications, offer a mechanism for tuning the electrical and optical properties. Such heterostacks have been demonstrated using serendipitous and low-throughput mechanical exfoliation and hand-stacking techniques. However, if the potential of such stacks is to be realised, industry-relevant processes must be developed and optimised.

Chemical vapour deposition (CVD) is a scalable technique which is used extensively for the growth of thin films in the semiconductor industry. In the case of 2D-materials synthesis, CVD offers improved scalability and throughput compared with mechanical exfoliation and improved material quality and scope for integration compared with liquid-phase exfoliation. While high-quality, large-area growth of graphene and assorted TMDs has been demonstrated by CVD, the synthesis of 2D-material heterostacks by analogous methods is still in its infancy, with only a few preliminary reports existing. Thus, further research and development in this area is required if these structures are to find use in real-world applications. This project will pioneer reliable and scalable synthesis methods for 2D-material heterostacks (and their constituent layers). The fundamental properties of said heterostacks will be investigated in great detail and novel characterisation methods developed, further driving academic research. The demonstration of optoelectronic devices from 2D materials, and their evaluation for different applications, will serve as a guide for industry (in particular ICT and energy) as feasible routes for the commercial development of 2D materials will be identified.

In addition to producing technologically relevant device prototypes, this project will develop non-destructive characterisation pathways for 2D-material heterostacks which will aid with understanding of the growth mechanisms for the constituent layers and the interfaces that form between them. Additionally, the effect of sandwiching organic molecules between 2D layers will be investigated, both for fundamental Raman spectroscopic studies and for tuning the properties of heterostacks.