Fully funded PhD position available in the School of Physics at University College Dublin (UCD).

Applications are invited for a PhD position at the School of Physics, University College Dublin, Ireland. The successful candidate will join the Computational Materials Research group led by Dr Nuala Caffrey (https://people.ucd.ie/nuala.caffrey).

Project Description:

Modelling multi-valent ion intercalation in layered MXene materials for next-generation energy storage

Multi-valent ion batteries, including Mg^{2+}, Ca^{2+}, Zn^{2+}, Al^{3+}-based batteries, are potentially safer, cheaper, and have higher energy densities than those of commercial Li-ion batteries (LIBs). However, finding electrode materials capable of reversibly intercalating these cations is a major stumbling block to progress in this area. While graphite is the most popular commercial rechargeable battery anode it is only suitable for Li-ion based batteries as its interlayer spacing is too small to accommodate larger ions.

This project will investigate the suitability of a recently discovered family of 2D materials, namely MXene materials, for this purpose. MXenes are formed through the selective chemical etching of a series of $M_{n+1}AX_n$ (i.e. MAX) phases, where M is an early transition metal, A is generally from group IIIA or IVA, X is either carbon or nitrogen and $n \in [1, 3]$. Several MXene phases have been experimentally produced, including Ti_3C_2, Ti_2C, Ti_3CN, Ta_4C_3, Nb_2C, V_2C and Nb_4C_3, with many more predicted theoretically.

Several experiments have shown that these materials have significant promise. For example, V_2CT_x MXene electrodes show one of the best performances among all reported cathode materials for Al batteries [1]. However, several open questions remain, including the exact nature of the intercalant and why certain MXenes are capable of intercalating particular cations but not others [2]. Answering these questions is crucial to the eventual use of MXene materials as next-generation multivalent-ion battery anodes.

The PhD student will use *ab initio* density functional theory (DFT) calculations to establish the intercalation mechanism of multivalent ions in layered MXene materials.

[1] ACS Nano 2017, 11, 11135
[2] Adv.Mater. 2021, 33, 2004039

The PhD position is fully funded, including a stipend of €18,000 per annum and a travel budget to present at international conferences.

Applicant Requirements:

Applicants must have at least a first or upper second-class honours primary degree and/or master's degree, or the equivalent, in a physics-related discipline. A solid background in condensed matter physics and an interest in computational methods is required.

Excellent written and oral communication skills are essential, including meeting the minimum English language requirements of UCD (http://www.ucd.ie/registry/admissions/elr.html).

Application Details:

Applicants should send (1) a CV, (2) a cover letter explaining their interest in the project topic and mentioning any relevant background and/or experience and (3) the names and contact details of 2 academic references to Dr. Nuala Caffrey (nuala.caffrey@ucd.ie) in a single PDF.

Application Deadline: 31st May 2023.

Short-listed candidates will be interviewed in mid-June, 2023.

Successful applicants must be formally enrolled by the UCD School of Physics by the start of September 2023.

Informal enquires welcome. Contact Dr. Nuala Caffrey at nuala.caffrey@ucd.ie.