

School of Physical Sciences Seminar

Location: SA217 and on Zoom

When: Thursday 17 Feb at 1pm

Speaker: Dr. Nuala M. Caffrey (School of Physics, UCD)

Topic: Between the Sheets: Adsorbents and Intercalants in 2D Layered Materials

Abstract: Two-dimensional (2D) solids have layer type structures in which strong covalent bonds provide in-plane stability while relatively weak dispersive forces hold the layers together. Intercalation involves the insertion of guest species, such as atoms or molecules, between the layers of a 2D solid. The effects of intercalation are not well understood for the majority of layered materials, and a range of different behaviours can be seen. In some cases, intercalation is a precursor to the complete exfoliation of the host material, whereas in others, intercalants remain between the layers and tune the behaviour of the host material.

In this talk, I will show how density functional theory and classical molecular dynamics calculations can be used to make the exfoliation process more efficient. This is achieved by determining which characteristics of individual intercalants are associated with an increased production of 2D monolayers. We find that energetic effects alone are not sufficient as a screening descriptor, and instead explicit interactions at the interface between the solvent and solute play a critical role.

I will also discuss how atomic intercalation can also be used to induce structural or electronic phase transitions in host materials, and how this depends on the nature of the host. For example, structural phase transitions in transition metal dichalcogenides (TMDs) and electronic transitions in layered carbides (MXenes) can be achieved using particular intercalation strategies.

The ability to tune the properties of layered materials in this way makes them highly promising for novel multi-valent battery electrodes, 2D electronics and highly efficient catalysts.

Everyone welcome!

If you cannot join in-person, please use the Zoom link:

<https://dcu-ie.zoom.us/j/99145308425?pwd=WjdLUE5xSDBLS3p5Q216UFd3WHkyUT09>

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