Meeting Global challenges for energy storage: Engineering discovery and development of MXene 2D-materials application in energy storage

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Location The Open University, Milton Keynes, United Kingdom

Full-time only.

Duration & Funding A 3 year 3 month studentship as part of EPSRC Doctoral Training Partnership; Stipend £18,622 per annum; Training grant £4,500

Application due date: Feb 26, 2024

Notification of shortlisting and online Interviews will be arranged promptly after the closing date

Final Funding Decision: Late April/early May 2024**.** This is part of a pooled EPSRC-DTP process, so the selected applicant will be put forward to a reviewing panel in April for final decisions. Applicants will be notified if they are selected, and will be informed of the panel decision afterwards.

Start date: October, 2024

Project-related enquiries: nicholas.power@open.ac.uk

Process-related enquiries: STEM-LHCS-phd@open.ac.uk

Research area/keywords: 2D-materials, MXene, MAX Phase, rechargeable batteries, supercapacitors.

Project background and description

With increasing global demand for mobile technology and subsequent demand for efficient and powerful energy storage systems to power them, significant advances in the development of batteries and supercapacitors are essential. Future batteries require extended performance beyond existing intrinsic limits which will theoretically

afford higher capacity and volumetric energy density at a lower economic and environmental cost. Such systems will require advances in new materials for the electrodes, electrolytes, and electrocatalysts to achieve the desired outcome in performance, reliability, safety, and economic viability, beyond what is currently feasible. Supercapacitors similarly require advances in new materials to increase the surface area (via nano-porosity for example) of electrodes and improved dielectrics to enhance their capabilities.

In this regard, MXenes[1], 2D nanomaterial derivatives of MAX phase[2,3,4] materials (early transition metal carbides or nitrides), are a family of such new advanced versatile materials[5] that can provide a unique 2D morphology, chemical composition, and surface and conductance properties, that can theoretically address many of the challenges faced in battery and supercapacitor development[6].

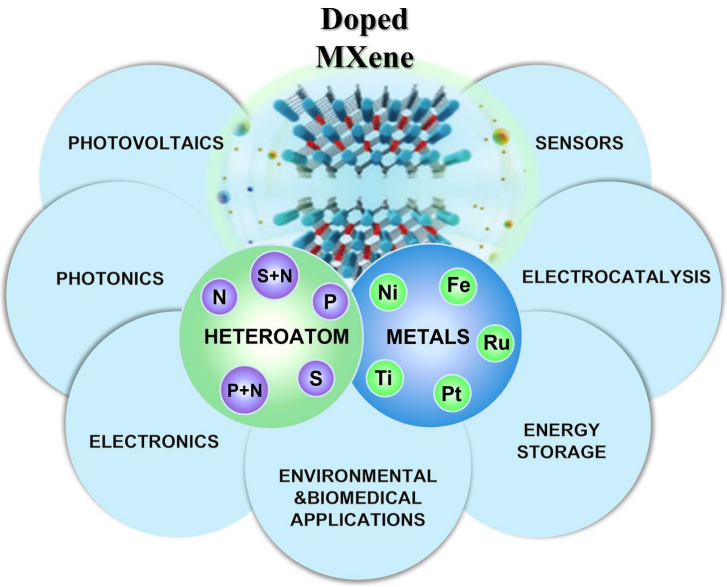

Figure 1. Schematic for the potential applications of doped MXenes using various metals and/or heteroatoms[6].

Aims: The main aim is to explore, design, and produce a targeted range of new unreported doped MAX Phase and MXenes using the methodologies described, and assess their potential for exploitation of their physico-chemical, electronic, and catalytic properties, for application in advancing development of energy storage systems. Doping of 2D materials can facilitate fine tuning of the physico-chemical properties of the 2D materials for energy storage including tuning the interlayer structure and surface area, improve electrochemical stability, and reduce charge transfer resistance for example.[6] The as-prepared materials and composites will then undergo electrochemical characterisation and explored and tested in application.

Facilities for materials characterisation at the OU include XPS, XRD spectroscopy, Raman, HRTEM, SEM, UV-Vis DRS, and FTIR spectroscopy (https://emsuite.stem.open.ac.uk) as well as collaborative access to the Surrey Ion Beam Centre for high end characterisation, such as Rutherford back scattering, TOF ERD etc. (https://uknibc.co.uk/SIBC/facilities.php) to understand the fundamental mechanism of surface and interface properties of the 2D systems**.**

References

1. Naguib *et al*., Two-Dimensional Nanocrystals Produced by Exfoliation of Ti_3AlC_2. *Adv. Mater.* 2011, 23, 4248–4253. https://doi.org/10.1002/adma.201102306
2. Deysher *et al.,* Synthesis of Mo_4VAlC_4 MAX Phase and Two-Dimensional Mo_4VC_4 MXene with Five Atomic Layers of Transition Metals*. ACS Nano. 14 (1): 204–217.* doi:10.1021/acsnano.9b0770
3. Eklund *et al*. The $M_{n+1}AX_n$ phases: Materials science and thin-film processing, 2010, Thin Solid Films, (518), 8, 1851-1878. https://doi.org/10.1016/j.tsf.2009.07.184
4. Li *et al*. Element Replacement Approach by Reaction with Lewis Acidic Molten Salts to Synthesize Nanolaminated MAX Phases and MXenes. *J Am Chem Soc* 2019;141, 4730–4737. https://pubs.acs.org/doi/10.1021/jacs.9b00574
5. Damptey *et al*. Surface functionalized MXenes for Wastewater treatment—a comprehensive review. *Global Challenges* 2022; 6:2100120. https://doi.org/10.1002/gch2.202100120
6. Dey *et al*., Doped MXenes—A new paradigm in 2D systems: Synthesis, properties and applications, *Progress in Materials Science*, Volume 139, 2023, 6, https://doi.org/10.1016/j.pmatsci.2023.101166

Eligibility

1. Applicants will ideally have a First Class or Upper Second undergraduate degree or Masters degree (or equivalent experience) in chemistry, materials science, solid-state physics/chemistry or other relevant scientific/engineering disciplines. Previous laboratory experience and knowledge of synthesis and characterisation techniques for inorganic materials and a broad interest in sustainable materials would be an advantage. Good numeracy, ICT, communication, and organisation skills are also desirable.

2. The student would be required to live in the UK and within commuting distance to The Open University campus in Milton Keynes.

We are committed to widening participation and awarding PhD studentships to a diverse community of applicants. We particularly welcome applications from under-represented groups. Equal Opportunity is University policy.

How to apply

Please check this page for application entry requirements: https://www.open.ac.uk/postgraduate/research-degrees/degrees-we-offer/doctor-of-philosophy-phd

Please submit to STEM-LHCS-PHD@open.ac.uk an:

- application form, and
- 2-page (A4) personal statement outlining your suitability for the studentship, what you hope to achieve from the PhD and your research experience to date

You do not need to submit a research proposal.

Information and the application form is found here: https://www.open.ac.uk/postgraduate/research-degrees/how-to-apply/mphil-and-phd-application-process. Note that as part of the application form, you will be asked to submit further documents (CV, degree transcripts, IELTS test scores where English is an additional language, etc.)