SHS produced high – entropy MXenes

Summary

The project aims at radically new and far beyond the state-of-the-art platform for the preparation of high-entropy MAX phases and their 2D counterparts (high-entropy MXenes) with targeted functionalities unleashing their potential for energy storage. The overall goals are (i) to prepare novel high-entropy MAX phases of high purity with the help of an energy-saving self-propagating high-temperature synthesis (SHS), and (ii) to develop 2D high-entropy MXene nanosheets of high conductivity, high flexibility, extended lifetime and electrochemical capacitance. The project addresses the following research questions: What are the main expected benefits and challenges of using SHS approaches for MXenes production? What is the most suitable precursor material and alternative concepts to mitigate combustion synthesis conditions? How to control the heating rate of reagents in the combustion wave and the post-combustion process? How to control a crystal structure and to facilitate subsequent delamination process of high entropy MXenes?

Research field:	Production and materials engineering, robotics, transport and logistics
Supervisors:	Prof. Dr. Irina Hussainova Sofiya Aydinyan
Availability:	This position is available.
Offered by:	School of Engineering Department of Mechanical and Industrial Engineering
Application deadline:	Applications are accepted between October 01, 2024 00:00 and October 25, 2024 23:59 (Europe/Zurich)

Description

The research

The advent of high-entropy MAX/MXenes with their mechanical properties, elevated temperature resistance and high chemical stability is poised to yield new advancement in the performance of energy storage and conversion technologies. Recent developments in fuel cells, batteries, supercapacitors, and hydrogen storage systems already point to future directions and new energy-related technologies that can be enabled by the application of HE MAX and MXenes. Based on these criteria, combinations of the early transition metals will be considered: Ta, Nb, Ti, V, Mo, Cr, Hf.

The motivation for this work is the urgent need in a knowledge-based design of high-entropy MXenes, possibility of facile synthesis of high-entropy MXene precursors by SHS method, development of a technological route for the scale-up fabrication thereof.

The goal of this PhD project is to examine the use of SHS approaches to fabrication of high-entropy MXene with tailored physicomechanical and electrochemical characteristics for energy storage applications, which are beyond reach with conventional approaches.

Specifically, the project should carry out computational studies based on first principle calculations and thermodynamics, quantify thermodynamic stability of target systems for the proper selection of the elements and the formation of a favorable single solid solution phase in high-entropy MAX and MXenes; perform preliminary SHS experiments taking into account the effect of synthesis temperature, duration, cooling mode on microstructures, phase composition and properties of the as-synthesized laminated powder and its 2D counterpart; develop strategies of tuning of combustion wave; design SHS route for producing high-entropy MAX of laminated microstructure and desired composition from M1M2M3M4M5-Al(Si)-C(N) (M is a transition metal) element combinations; design a green path for MXene preparation etching in HF-free solution.

Responsibilities and (foreseen) tasks

- Computational design of the thermodynamically stable system;
- Self-propagating high-temperature synthesis of high-entropy MAX phases of the selected composition;
- Optimization of process parameters and development combustion synthesis technology;
- Development of cost-effective and waste-free strategies for 2D MXene preparation;
- Characterization of the produced materials (microstructure, composition, mechanical properties);

- Assessment of the potential methodological and technical risks, provide timely dissemination and secure exploitation of results, provide public engagement and outreach;
- Contribute to the organization of research and practitioner workshops where project findings are presented

Applicants should fulfil the following requirements:

- a master's degree in Materials Sciences or Chemistry (preferably in metals and ceramics; materials chemistry; and powder metallurgy)
- skills and experience in computational design
- some experience in materials microstructural characterization (optical microscopy, SEM, XRD etc) by use of quantitative methods
- a clear interest in the topic of the position
- excellent command of English
- strong and demonstrable writing and analytical skills
- capacity to work both as an independent researcher and as part of an international team
- capacity and willingness to provide assistance in organizational tasks relevant to the project

The following experience is beneficial:

- Experimental and/or theoretical knowledge of SHS processes
- Experience/ knowledge of ThermoCalc® or any other thermodynamic software and first principal calculations
- Experience with optical and scanning electron microscopy
- Previous experience working with high-entropy materials and/or MAX phases

<u>The candidate should submit a research plan for the topic, including the overall research and data collection strategy. The candidate can expand on the listed research questions and tasks, and propose theoretical lenses to be used.</u>

We offer:

- 4-year PhD position in one of the largest, most internationalized and leading social science research centers in Estonia with a large portfolio of ongoing pan-European and national public administration, digital governance and innovation studies projects
- The chance to do high-level research in one of the most dynamic digital government contexts globally. Individual development and training opportunities.
- An informal and inclusive international working environment, green campus approach, a flexible schedule and modern office facilities located in Tallinn
- Opportunities for conference visits, research stays and networking with globally leading universities and research centers in the fields of public administration, innovation studies and digital government

About the department

The department of Mechanical and Industrial engineering focuses on the engineering side of self-driving vehicles, developing new material systems and coatings and additive manufacturing developments. The curriculums on Bachelor, Masters and Doctor level have hundreds of graduates each year.

The Materials Engineering Research Centre in our department brings together leading scientists and PhD students to form a vibrant and collaborative environment for research into materials engineering. The centre has expertise in materials (particularly powder materials, thin and thick coatings, materials characterisation), materials technologies (powder metallurgy, surface engineering, joining technology etc.) and related industrial applications.

We also provide engineering services for industry and our partners, starting with modelling and finishing with production optimization. TalTech houses state-of-the-art powder metallurgy and additive manufacturing laboratories, plus laser, optical, metrology and chemical labs and equipment – the ideal environment for world-class materials development.

Additional information

For further information, please contact Prof. Irina Hussainova (Irina.hussainova@taltech.ee) and Dr. Sofiya Aydinyan (sofiya.aydinyan@taltech.ee) or visit https://taltech.ee/en/department-mechanical-and-industrial-engineering

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