Project Description for UiO:Energy Scholarship Summer 2021

Project Title: Synthesis and Characterization of Novel Zn_2NF Quantum Dots for Photocatalysis
Number of projects: One
Supervisors: Anja Olafsen Sjåstad (main supervisor), Helmer Fjellvåg (co-supervisor)

Background

The size-tunable optoelectronic properties of inorganic semiconductors make them a key component of technologies that harvest renewable energy, such as photovoltaic cells[1] and photocatalysts[2]. Yet, the most studied and used semiconductors in existing technologies contain toxic elements, including cadmium[3] and lead[4]. In order to be suitable for environmentally-friendly large-scale manufacturing, the semiconductor must be composed of materials that are widely available, inexpensive and non-toxic. The development of such compositions is an active field of research.

The bandgap of the semiconductor is an important parameter for the conversion of solar light into chemical energy. The size of the bandgap is primarily determined by the electronegativity difference between the cation and anion of the semiconductor, as well as the extent of their valence orbital overlap[5]. Moreover, the bandgap also depends on particle size[6], making it an additional parameter in bandgap tuning. When a semiconductor is smaller than the exciton Bohr radius they are in the quantum size regime, and are popularly called quantum dots.

Lingampalli et al. recently reported the preparation of Zn_2NF, a bulk mixed anion metal nitride-fluoride semiconductor[5]. All three components of the semiconductor, zinc, nitrogen and fluorine, fulfill the criteria for environmentally-friendly large-scale manufacturing. The synthesis of Zn_2NF was made possible by the aliovalent substitution of N^{3-} and F^{-} anions in place of O^{2-} anion of ZnO. While ZnO is a wide bandgap semiconductor[5] that has band to band transitions in the ultra violet (UV) spectrum, Zn_2NF is a small bandgap semiconductor with band to band transition in the visible light spectrum[5]. As a consequence, when exposed to sunlight, Zn_2NF works as an active photocatalyst in the splitting of water, thus producing the energy carrier hydrogen gas[5].

In photocatalysis, as the particle size decreases, the surface area increases, multiplying the number of active sites. In addition, the bandgap of the material can be tuned and a specific particle size can maximize the reaction yield. Thus, if applied at the nanoscale, the photocatalytic activity of Zn_2NF can be significantly amplified[7], increasing the number of potential applications, ranging from water splitting[3,4] to pollutant degradation from water sources[8].

The objective of this project is to establish a method for controlled quantum dot-synthesis of Zn_2NF by adapting the protocols published by Taylor et al.[9] and Ahumada-Lazo et al.[10] for synthesizing Zn_3N_2 nano-sized semiconductors. Then, the bandgap of the Zn_2NF quantum dots will be evaluated relative to bulk Zn_2NF. Finally, the Zn_2NF quantum dots will be characterized using powder X-ray diffraction (XRD) and scanning electron microscope (SEM) equipped with an energy-dispersive X-ray spectroscopy (EDS).

Research Objectives
1) To establish a method for synthesis of Zn_2NF quantum dots.
2) To evaluate the bandgap of the Zn_2NF quantum dots relative to bulk Zn_2NF, and to characterize the phase content and particle size of the synthesized Zn_2NF quantum dots.

Expected Project Outcomes
- Develop a protocol for synthesis of Zn_2NF quantum dots.
- Produce core data for a scientific paper that can be finalized and published in cooperation with a PhD student in the NAFUMA research group.
- Make a presentation of the results for the NAFUMA research group.

Methods
Synthesis
Colloidal synthesis routes at inert conditions will be performed using Schlenk lines and gloveboxes. This enables the exploitation of the LaMer's theory to separate the homogeneous nucleation step from the growth phase resulting in monodisperse particle size[11]. In order to establish a method for controlled quantum dot-synthesis of Zn_2NF, we will adapt the protocols published by Taylor et al.[9] and Ahumada-Lazo et al.[10] for synthesizing nano-sized semiconductors of Zn_3N_2.

Characterization
Phase content, particle size, and bandgap of the obtained quantum dots will be characterized by powder XRD, SEM equipped with an EDS and UV-Vis absorbance spectra.

Candidate Background
The preferred candidate has previous experience in quantum dot synthesis, XRD and SEM. In addition, the candidate must have strong academic credentials, research experience and an interest in developing nanomaterials for sustainable energy systems.

Project Period
The preferred project period would be six weeks of full-time research from 7 June 2021 to 18 July 2021.

Future work
The NAFUMA research group is currently pursuing a project studying novel compounds with mixed anion-systems, such as Zn_2NF, for potential applications in renewable energy. Moreover, NAFUMA is applying for funding from “Fellesløftet” for a multidisciplinary study on the fundamentals of new semiconductors, along with the research groups LENS and Structure Physics. The project outlined in this proposal will be developed as part of this ongoing research.

References

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