Final Report of Åforsk Project (Ref. nr. 22-206):

A new research avenue for glassy materials: the next generation solid-state Na-ion batteries

1 Summary

In this project, we investigate energy materials with a particular focus on Na- and Li-based glasses and the role of structural disorder in determining their properties. The work was carried out through atomistic simulations: we performed Density Functional Theory (DFT) calculations to examine the electrochemical stability of a glassy electrolyte in contact with Li metal. Our results identify a mechanism in which molecular oxygen impurities within the glass matrix enhance the electrolyte's electrochemical stability. The amorphous structure of the glass has also been analyzed and characterized. A manuscript is currently in preparation.

We additionally carried out DFT simulations to study the interfacial properties of an all–solid-state lithium battery system consisting of lithium metal as the anode and Li_3OCl as the solid electrolyte. The investigation evaluates the structural properties, electronic structure, and electrochemical stability of the Li—Li_3OCl interface. Our findings show that this interface is thermodynamically stable against lithium metal, indicating favorable interfacial compatibility. Furthermore, no significant electronic states appear at the Fermi level, confirming the absence of electronic conductivity across the interface. However, despite the stable interface, bulk Li_3OCl exhibits limited lithium-ion mobility.. A manuscript is currently in preparation.

In addition, we explored two-dimensional materials, including a type-II $MoSi_2N_4$/As an der Waals heterostructure, Rashba spin textures in an asymmetric Bi_2O_2Se monolayer, and a hydrogen-enriched vanadium-sulfide-hydride Janus monolayer for applications in solar cells, spintronic devices, and Li-/Na-/Ca-ion batteries, respectively. The intrinsic asymmetry of these systems offers promising technological opportunities across diverse fields. Here, we additionally carried out Molecular Dynamic simulations to investigate the stability of these systems.

The calculations in these works were carried out by the PI in collaboration with colleagues at KTH and international partners. The computations were enabled by resources provided by the National Academic Infrastructure for Supercomputing in Sweden (NAISS), partially funded by the Swedish Research Council, Sweden through grant agreement no. 2022-06725. These resources were granted to the PI. In cases where experimental work was included, it was performed in collaboration with research groups in England and Germany.

The project has resulted in three published papers in high-impact journals, three manuscripts currently under review in leading scientific journals, and five additional manuscripts in preparation for submission. Thanks to the support of Åforsk, this work has opened new research avenues in glassy materials and other relevant two-dimensional materials for energy-storage systems.

2 Publications

Below is a list of publications produced between 2022 and 2025, whether published, under review, or in preparation, that contain the appropriate acknowledgement to Åforsk.

2.1 Peer-reviewed

1. *Theoretical prediction of a high-performance two-dimensional type-II $MoSi_2N_4$/As vdW heterostructure for photovoltaic solar cells*
   D. Singh, N. Khossossi, **R. Lizárraga** and Y. Sonvane. (Impact Factor: **9.0**)

Renewable Energy **237**, 121802 (2024)

2. *Voltage-Gated 90° Switching of Bulk Perpendicular Magnetic Anisotropy in Ferrimagnets*
Z. Xiao, R. Xie, F. Maccari, P. Klaßen, B. Eggert, D. Wang, Y. Dai, **R. Lizárraga**, J. Lill, T. Helbig, H. Wende, K. Kummer, K. Ollefs, K. P. Skokov, H. Zhang, Z.Quan, X. Xu, R. Kruk, H. Hahn, O. Gutfleisch and X. Ye. (Impact Factor: **15.6**)
ACS Nano **19**(6) 6021–6032 (2025)

3. *Hydrogen-enriched vanadium-sulfide-hydride Janus monolayer unlocks high-performance anodes for Li/Na/Ca-ion batteries*
R. P. Jadav, D. Singh, **R. Lizárraga**, R. Ahuja and Y. Sonvane (Impact Factor: **9.8**)
J. Energy Storage **141** 119239 (2026)

4. *Tuning Rashba Spin Textures in Asymmetric Bi_2O_2Se Monolayer for spintronic applications* D. Singh, Y. Sonvane, R. Lizárraga
Under review in npj — 2D materials and applications.

5. *A Dynamic Hydrogen-Bonded Organic Framework with Giant ON-OFF Birefringence*
C. Halliwel, M. E.J. Elsegood, S. Fowler, K. Jolley, D. Singh, **R. Lizárraga**, A. Fernandez
Under review in Advanced Functional Materials.

6. *A universal upcycling process for both single and mixed blends of textile fiber blends*
K. H. Zangana, C. Prajapati, D. Engstrom, J. Burgess, N. Heath, S. Gao, B. Benyahia, J. D. Holmes, D. Singh, **R. Lizárraga** and A. Fernandez.
Under review in Advanced Materials.

2.2 In preparation

i. *Electrocatalytic Performance of Hydrogen Enrich 2H–VSH Janus cathode for Sodium–Sulfur Batteries*
R. P Jadav, D. Singh and **R. Lizárraga**, R. Ahuja, Y. Sonvane

ii. *Highly selective and sensitive lung cancer molecules de- tection by 2D C2N monolayer*
D. Singh and R. Lizárraga

iii. *Redox activity of trapped O_2 molecules controlling the electrochemical stability of glassy electrolytes*
D. Singh, L. Tian, and C. M. Araujo, and **R. Lizárraga**
Under preparation.

iv. Interfacial phenomena in all-solid-state batteries
D. Singh, L. Tian, and C. M. Araujo, and **R. Lizárraga** Under preparation.

2.3 Minestones

- A bachelor thesis: "Quantum mechanical modelling and electrochemical stability of sodium based glassy electrolyte for all-solid-state batteries" by Carolina Falk and Linnéa Johansson. (10 credits / 15 HE credits).
Supervision: **Raquel Lizárraga**, KTH Kungliga Tekniska Högskolan. (2022).

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- The principal investigator became Docent in the subject of atomistic simulations for energy storage materials in 2023 (KTH). The subject of the current investigation has been used to prepare the docent application and lecture.
- Elements of this project have been integrated into Master's courses at KTH and were also used to support a high-school research project conducted in 2024 at KTH through the Rays for Excellence mentorship program.