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S E M I N A R
on
Semiconductor Physics and Nanotechnology

Mo, 22.09.2025, 10:15 Uhr,

Seminar in person in the Electrical engineering lecture hall *or* via Zoom

"Structure–Property Relationships Across Material Dimensions: Semiconductor Quantum Dots, MXenes, and Bulk Cathode Materials"

Dr. Arup Chakraborty

Materials Modelling Laboratory, Department of Materials, University of Oxford, UK

Achieving net-zero emissions requires both renewable energy and sustainable storage solutions, and understanding structure–property relationships is key to advancing these materials. This talk highlights how computational modelling, combined with experiments, reveals fundamental insights across different material dimensions.

First, I will discuss bulk cathode materials for rechargeable batteries, focusing on how dopants stabilize Li-ion and Na-ion layered oxides by mitigating oxygen loss and phase transformations.[1,2] These atomistic insights provide guidance for designing robust energy storage materials.

Next, I will move to two-dimensional MXenes, showing how Ti_3C_2-based sheets act as selective ion-transport membranes in zinc-halide batteries.[3,4] Finally, I will discuss zero-dimensional semiconductor quantum dots in photovoltaics, where computational studies clarify the effects of quantum confinement and strain.[5]

Together, these examples demonstrate how structure–property relationships evolve from bulk to 2D to 0D quantum-confined systems, advancing next-generation energy technologies.

References

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3. A. Roy, A. Chakraborty, G. Valurouthu, Y. Zhang, G. Bergman, N. Shpigel, M. S. Islam, D. Mandler, Y. Gogotsi. 2D MXene-based membranes for the suppression of halide crossover in Zn-halide batteries. *ACS Appl. Mater. Interfaces*, 17, 49400–49408 (2025).
4. N. Shpigel, A. Chakraborty, F. Malchik, G. Bergman, A. Nimkar, B. Gavriel, M. Turgeman, C. N. Hong, M. R. Lukatskaya, M. D. Levi, Y. Gogotsi, D. T. Major, and D. Aurbach. Can anions be inserted into MXene? *J. Am. Chem. Soc.* 143, 12552 (2021).
5. A. Chakraborty, B. Das, I. Dasgupta, Unlocking the electronic, optical and transport properties of semiconductor coupled quantum dots using first-principles methods; *Int. J. Quantum Chem.*, e27101, 1-11 (2023).

Zoom – Link:
https://zoom.us/j/96375934537?pwd=RTlKTWhSdzRHU211YTY1bGFxTUtpZz09
Meeting-ID: 963 7593 4537
Kenncode: =r=4YQ