東京大学大学院工学系研究科　総合研究機構

結晶界面工学研究室

Crystal Interface Laboratory, The University of Tokyo

Crystal Interface Lab. Seminar Series

"Understanding extended defects in energy materials through first-principles calculations and electron microscopy"

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Semiconducting materials find diverse applications in areas such as microelectronics, lighting and renewable energy. For energy applications such as photoelectrochemical cells, photovoltaics and themoelectrics significant effort is now focused on the discovery and optimisation of semiconductors to improve performance and materials sustainability. In practice such materials are often polycrystalline with extended defects such as grain boundaries and dislocations playing a decisive role in their properties. For example, grain boundaries in solar absorbers often cause enhanced non-radiative electron-hole recombination reducing the performance of photovoltaic devices. While the role of extended defects on mechanical properties is relatively well understood their impact on electronic and optical properties is far less clear and challenging to probe experimentally. In this talk, I will present some of our recent work on modelling the structure and properties of extended defects in a range of energy materials of practical and fundamental interest using first principles methods. These materials include titanium dioxide [1-4], formamidinium lead iodide [5], antimony selenide [6,7,] bournonite and enargite [8].

References

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[3] G. Schusteritsch et al, Nano Lett. **21**, 2745 (2021)
[4] J. Debgupta et al, J. Phys. Chem. C **127**, 660 (2023)
[5] K. P. McKenna, ACS Energy Letters **3**, 2663 (2018)
[6] R. E. Williams et al, ACS Appl. Mater. & Inter. **12**, 21730 (2020)
[7] K. P. McKenna, Adv. Electron. Mater. **7**, 2000908 (2021)
[8] O. M. Rigby et al, J. Appl. Phys. **132**, 185001 (2022)

Main meeting room at Institute of Engineering Innovation

工学部総合研究機構９号館１階　大会議室

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