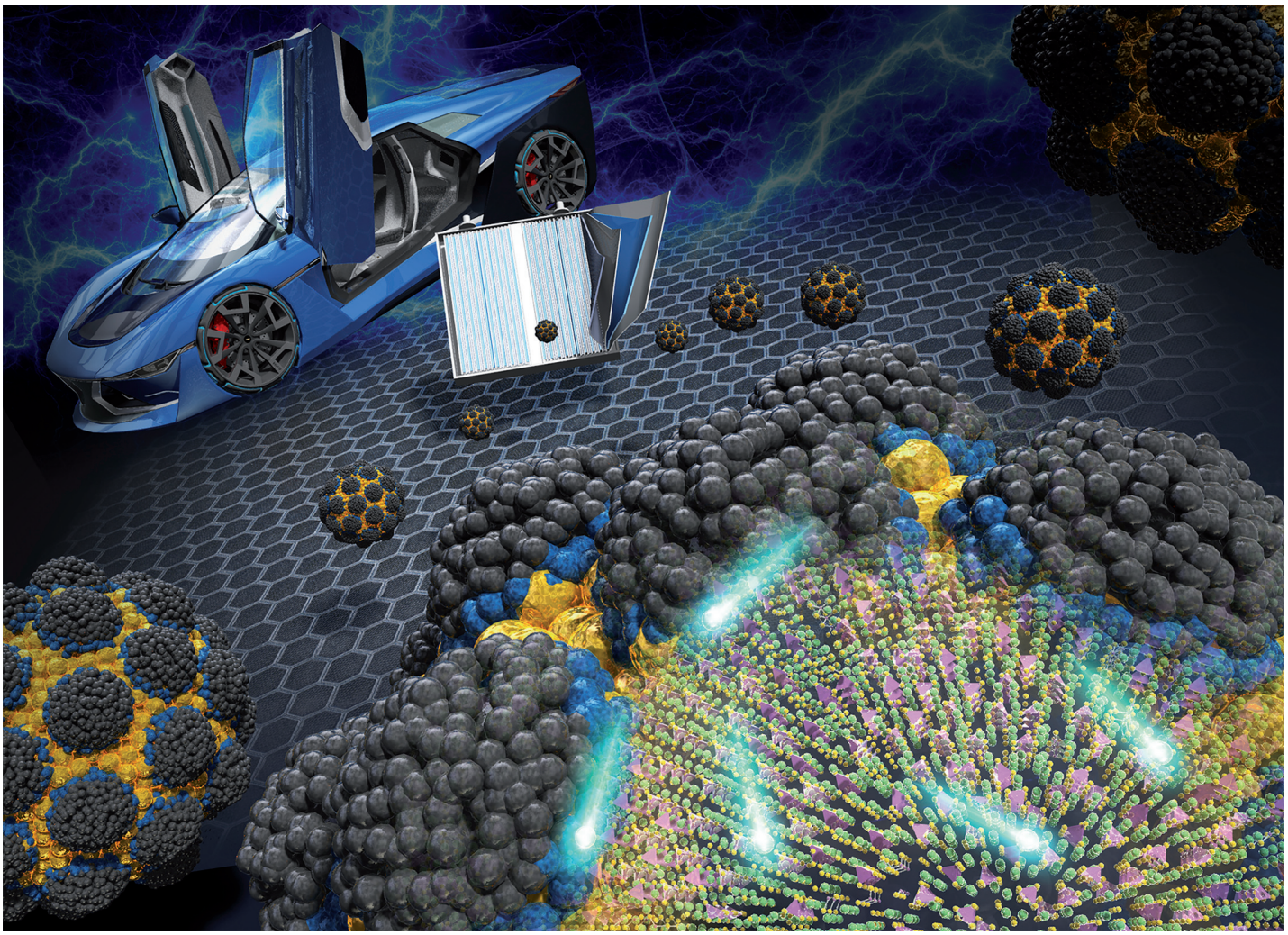
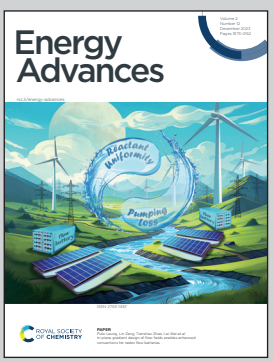


Showcasing research from Professor Shyue Ping Ong's laboratory, Department of NanoEngineering, University of California San Diego, USA.

Lithium dynamics at grain boundaries of β-Li_3PS_4 solid electrolyte

β-Li_3PS_4 (β-LPS) is a promising solid electrolyte for all-solid-state Li ion batteries due to its good Li ionic conductivity, good formability, and low processing cost. In this work, the Li ion transport in tilt and twist grain boundaries as well as amorphous/crystal interfaces of β-LPS was systematically investigated by performing large-scale molecular dynamics simulations with a highly accurate moment tensor interatomic potential. It was determined that the Li ion conductivities at the grain boundaries and amorphous/crystal interfaces are 1–2 orders of magnitude higher than that in the bulk crystal.

As featured in:



See Shyue Ping Ong *et al.*, *Energy Adv.*, 2023, **2**, 2029.

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