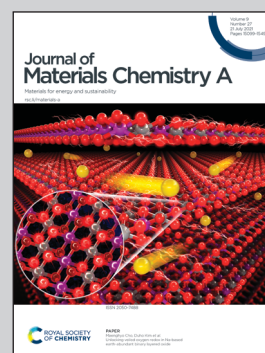


Showcasing research from Prof. Yoshitaka Tateyama's group at National Institute for Materials Science (NIMS), Japan.

Tuning the performance of a Mg negative electrode through grain boundaries and alloying toward the realization of Mg batteries

The effects of the grain boundaries (GB) and surfaces on the Mg electrode performance and how the different alloying elements tune the GB characteristics are comprehensively explored *via* first-principles calculations. Mg atoms at [0001] (10 $\bar{1}$ 0) tilt GB and (11 $\bar{2}$ 0) surface are preferentially stripped during discharge, resulting in a "pit-type" morphology. Alloying with Ca increases the GB amount and the current density. These results also suggest a new electrochemical energy diagram extending from the conventional electrochemical theory.

As featured in:



See Hong-Kang Tian,
Yoshitaka Tateyama *et al.*,
J. Mater. Chem. A, 2021, **9**, 15207.