



Showcasing research from NAFUMA-Battery laboratory (Prof. Alexey Y. Kozlov's group), Centre for Material Science and Nanotechnology, Department of Chemistry, University of Oslo, Oslo, Norway.

Replica exchange molecular dynamics for Li-intercalation in graphite: a new solution for an old problem

In the present article, we studied a new solution for explaining the staging mechanism of Li storage in graphite. To overcome the computational limitations for modeling the Li intercalation, we deployed replica exchange molecular dynamics simulations previously not used to analyze active battery materials. We focused our work on analyzing the local Li arrangement in graphite, considering three main characteristics: Li distribution, graphite stacking mode, and spacing between graphene layers. The observed tendency for Li clustering led to dynamic local structures that approximate the staging models.

As featured in:



See Heesoo Park, David S. Wragg and Alexey Y. Kozlov *et al.*, *Chem. Sci.*, 2024, **15**, 2745.