



Highlighting a study on the key lattice dynamic factors for enhanced ionic conductivity of protonated antiperovskite electrolytes from the In-silico advanced materials Design (IamD) laboratory of Prof. Hong Zhu in the UM-SJTU Joint Institute of Shanghai Jiao Tong University.

Enhanced ionic conductivity of protonated antiperovskites *via* tuning lattice and rotational dynamics

Combining multiple factors, the overall soft lattice and the soft rotation mode of anion groups, which is correlated to Li migrations, can effectively optimize the Li ion conductivity in protonated antiperovskite electrolytes, which was supported by density functional theory calculations.

As featured in:



See Hong Zhu *et al.*,
J. Mater. Chem. A, 2023, **11**, 6157.