

Abstract Submitted
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Cluster-inspired Superionic Conductors HONG FANG, PURU JENA, Virginia Commonwealth University — Superionic conductors with desirable properties hold the key to the development of next generation of rechargeable metal-ion batteries. In this study, we report a new family of superionic conductors composed by clusters based on the antiperovskite fast-ion conductors. The new lightweight conductor shows larger electrochemical stability window and favorable thermal and mechanical properties, while maintain a high Li^+ -ion conductivity at room temperature and a low activation energy. We reveal the conduction mechanism of the material by identifying the relation between the orientational symmetry of the cluster rotors and the potential surface felt by the lithium ion. We also find that the mixed phase of the new conductors show further enhanced conductivity.

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