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Computational search for novel Zn-ion conductors—a crystallochemical, bond valence, and density functional study

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Zinc-based batteries have been a recurring theme throughout history, from Volta's pile, the Daniell and Leclanché elements to powering modern space vehicles. To date, no rechargeable all solid-state Zn-ion battery has been commercialized. Therefore, we intended to contribute to increasing the number of available Zn-ion conductors for such batteries. We used a stepwise algorithm (Voronoi partition, BVSE, and DFT) to identify compounds from the ICSD prone to Zn-ion conductivity.

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