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Simultaneous Blocking of Minority Carrier and High Energy Phonon in p-type Skutterudites

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### **ACCEPTED MANUSCRIPT**

#### Simultaneous Blocking of Minority Carrier and High Energy Phonon in p-type

#### Skutterudites

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**Abstract:** Skutterudites are among the most promising thermoelectric materials. However, the strong bipolar effects and a lack of high energy phonon scattering make the thermoelectric performance of p-type skutterudites far below that of n-type skutterudites. Here, we reveal that the distribution of cations spatially fluctuate in p-type skutterudites, leading to a band edge fluctuation with small valence-band offsets, multi-scale strain field fluctuation, and formation of nanostructures. It further results in a significant suppressed bipolar effect, and wide-frequency spectrum phonon scattering. A 38% enhanced power factor and reduced lattice thermal conductivity approaching to the theoretical minimum at 723 K lead to a remarkable theoretical conversion efficiency of 13.3%, reaching the highest records in p-type lead-free thermoelectric materials. Our results provide a new thought to realize high performance in polynary thermoelectric materials.

Keywords: filled skutterudites, selective scattering, bipolar effect, cation fluctuation

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