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Theoretical survey of doped sodium cobaltate and strategies for enhancing the thermoelectric performance[1] M. HUSSEIN N. ASSADI, HIROSHI KATAYAMA-YOSHIDA, Osaka University — Doped Na_xCoO_2 is suitable for highly efficient thermoelectric conversion at ≈ 1000 K. However, due to complex lattice structure and strong correlation effects, atomistic understanding of dopant's influence is challenging to resolve experimentally. We examined a wide range of dopants' electronic structures using density functional method. We found that dopants like Mg, Ba, Sr, Au and Eu always substitute Na for all Na concentrations. In contrast, dopants like Ni, Bi, W, Sb and Sn always substitute Co regardless of Na concentration. Furthermore, there is a third class of dopants like Cu and Y that substitute Na for $x \leq 0.5$, but for higher Na concentrations, they substitute Co. In the case of Mg_{Na}, we could experimentally verify Mg's local chemical environment using Raman spectroscopy therefore validating the theoretical results. The implication of Na-substituting dopants on thermoelectric performance is the immobilization of Na ions which behave similar to ionic liquid in pristine Na_xCoO_2. This immobilization reduces the resistivity by improving the mobility of carriers and thus enhancing the thermo-power.

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