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Thermoelectric properties of the layered rhodates K_xRhO_2 and Na_xRhO_2

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We discuss the structural as well as thermoelectric properties of the layered compounds K_xRhO_2 in comparison to isostructural and isovalent Na_xCoO_2. The optimized structure of $K_{1/2}RhO_2$ exhibits a remarkable deviation of the c/a ratio from the experimental result as well as from c/a ratios of related compounds. This indicates that a hydrated phase of K_xRhO_2 exists and the experimental structure determination refers to this hydrated phase. The calculated Seebeck coefficient of pristine $K_{1/2}RhO_2$ amounts to 50 μV/K at 300 K, which is close to the experimental value 40 μV/K. Importantly, we observe high values for the Seebeck coefficient and power factor for hydrated K_xRhO_2 in the whole temperature range from 0 to 700 K. At 100 K, we find for hydrated $K_{7/8}RhO_2$ a value $Z = 3\cdot10^{-3}\ K^{-1}$, which is the highest power factor observed at this temperature. It exceeds also the exceptionally high value of $Na_{0.88}CoO_2$ by more than 50%. Our results, hence, demonstrate that hydration is an effective approach to modify the lattice parameters and, as a result, enhance the thermoelectric performance.

The Na_xRhO_2 oxides are found to form a new class of materials with exciting thermoelectric features, even outperforming the 2H phases of the K_xRhO_2 system. In the latter the optimal thermoelectric performance is achieved at low temperature, whereas the modified stacking of the atomic layers in the 3R phases of Na_xRhO_2 results in a reduced interlayer coupling and, in turn, in a dramatically enhanced thermoelectric response in the technologically relevant high temperature range. We find that Na vacancies in Na_xRhO_2 avoid clustering and that the RhO_6 octahedra are modified depending on the amount of Na deficiency. Analysis of the induced changes in the DOS close to the Fermi level indicates that the $Rh^{3+\delta}$ $d_{3z^2-r^2}$ states control the transport properties of the compounds. A substantial figure of merit of 0.35 at 580 K is found in hydrated $Na_{0.83}RhO_2$ due to the enhanced effective mass of the charge carriers. In general, the figure of merit can be further increased by reduction of the Na vacancy concentration to increase the resistivity.

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