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Enhanced thermoelectric properties via oxygen non-stoichiometry in La_2NiO_4 and $SrTiO_3$ VICTOR PARDO, ANTIA S. BOTANA, Departamento Fisica Aplicada, Universidade Santiago de Compostela, Spain, PAUL M. BACH, VICTOR LEBORAN, FRANCISCO RIVADULLA, CIQUS, Universidade Santiago de Compostela, Spain, DANIEL BALDOMIR, Departamento Fisica Aplicada, Universidade Santiago de Compostela, Spain — We present the results of transport properties calculations and experiments on various oxides. A large enhancement of the thermoelectric properties is predicted[1] via ab initio calculations for $La_2NiO_{4+\delta}$, with electronic-only thermoelectric figure of merit (zT) values exceeding unity for oxygen excess $\delta \leq 0.10$. The effects of lattice strain (caused, e.g. by growth of thin films on different substrates) enhance even further the thermoelectric response. A similar result is obtained at very low electron-doping in bulk $SrTiO_3$ via oxygen removal. This is analyzed experimentally via thermal annealing that depletes oxygen ($\sim$ 1 oxygen vacancy per 10^6 unit cells). In both these systems, the increase in conductivity reached in the metallic limit retains a large thermopower, with the corresponding enhancement of zT. In the case of $SrTiO_3$, experiments indicate[2] that such a small oxygen vacancy level reduces drastically the thermal conductivity by introducing random scattering centers. In the talk, we will discuss the electronic structure origin of the enhancement of the thermoelectric response and how this can be tuned. Results are general and applicable to other non-stoichiometric oxides.

[1]PRB 86, 165114 (2012).
[2]arxiv:1211.1615.

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