Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Dopant's chemical coordination: a path for engineering high performance thermoelectric sodium cobaltate[1] M. HUSSEIN N. ASSADI, HIROSHI KATAYAMA-YOSHIDA, Osaka University — Engineered $Na_{0.75}CoO_2$ is considered a prime candidate to achieve high efficiency thermoelectric systems to generate electricity from waste heat. Our recent experiments on Mg doped $Na_{0.75}CoO_2$ demonstrated 50% enhancement in power factor at ambient. This motivated us to theoretically analyze the mechanisms behind simultaneous improvement of interdependent Seebeck coefficient and electrical conductivity. For this, we comprehensively studied the electronic and crystallographic structure of $Na_{0.75}CoO_2$ doped with 5 elements Mg, Sb, Zn, Ni and Eu. These elements represent wide variety of electronic configurations such as open d and f shells, closed d and s shells, combined with great variation in atomic mass. Systematic density functional calculations showed that the Ni and Zn were more stable when substituting Co with formation energy 2.35 eV, 2.08 eV. While Eu and Mg and Sb are more stable when it substitutes Na. In the case of Mg these results are consistent with Raman scattering measurement. This suggests that the doped Mg ions immobilize Na ions, reducing the resistivity by improving the mobility of carriers and thus enhancing the thermo-power.

[1]This work was supported by JSPS and Intersect.

M. Hussein N. Assadi
Osaka University

Date submitted: 15 Dec 2013 Electronic form version 1.4