

Supporting Information

Investigation of Thermoelectric Performance and Power Generation

Characteristics of Dual-Doped $\text{Ca}_{1-x}\text{RE}'_{x/2}\text{RE}''_{x/2}\text{MnO}_3$

($\text{RE}'/\text{RE}'' = \text{Dy, Gd, Yb, Lu}; 0.05 \leq x \leq 0.1$)

Rapaka S C Bose and Abanti Nag^{a)*}

*Materials Science Division, CSIR-National Aerospace Laboratories, Bangalore 560017,
India*

** Corresponding author : abanti@nal.res.in*

Table S1. Comparison of thermoelectric performances of CaMnO₃ with respect to doping and synthesis methodology

Synthesis methodology	Compositions	Power factor at 973 K ($\mu\text{Wm}^{-1}\text{K}^{-2}$)	Reference
Solid State Synthesis	Ca _{0.9} Yb _{0.1} MnO ₃	300	20
	Ca _{0.9} Dy _{0.1} MnO ₃	360	20
	Ca _{0.97} Bi _{0.03} MnO ₃	465	29
	CaMn _{0.98} Nb _{0.02} O ₃	120	30
	CaMn _{0.96} Ta _{0.04} O ₃	85	30
	CaMn _{0.99} W _{0.01} O ₃	340	31
	Ca _{0.8} Sr _{0.1} Yb _{0.1} MnO ₃	220	19
	Ca _{0.9} Yb _{0.05} Dy _{0.05} MnO ₃	345	23
	Ca _{0.96} Dy _{0.02} Bi _{0.02} MnO ₃	420	37
	CaMn _{0.96} Nb _{0.02} Ta _{0.02} O ₃	200	31
	Ca _{0.95} Yb _{0.05} Mn _{0.98} Nb _{0.02} O ₃	140	30
	Ca _{0.98} Lu _{0.02} Mn _{0.98} Nb _{0.02} O ₃	125	30
	Ca _{0.96} Gd _{0.04} Mn _{0.96} Nb _{0.04} O ₃	225	29
	Ca _{0.96} Bi _{0.04} Mn _{0.96} Nb _{0.04} O ₃	200	33
Co-precipitation	Ca _{0.96} Gd _{0.04} MnO ₃	310	22
Sol-gel Methodology	CaMn _{0.98} Nb _{0.02} O ₃	202	17
	Ca _{0.9} Yb _{0.05} Lu _{0.05} MnO ₃	580	This paper
	Ca _{0.9} Dy _{0.05} Lu _{0.05} MnO ₃	545	This paper
	Ca _{0.9} Dy _{0.05} Yb _{0.05} MnO ₃	560	This paper
	Ca _{0.9} Gd _{0.05} Lu _{0.05} MnO ₃	530	This paper
	Ca _{0.9} Gd _{0.05} Yb _{0.05} MnO ₃	475	This paper
	Ca _{0.9} Dy _{0.05} Gd _{0.05} MnO ₃	460	This paper

Figure S1

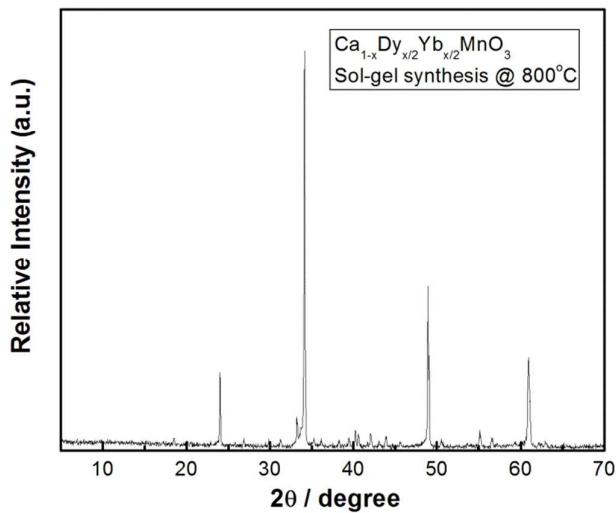


Figure S1. XRD pattern of sol-gel synthesized $\text{Ca}_{0.9}\text{RE}'_{0.05}\text{RE}''_{0.05}\text{MnO}_3$ after heat treatment of 800°C

Figure S2

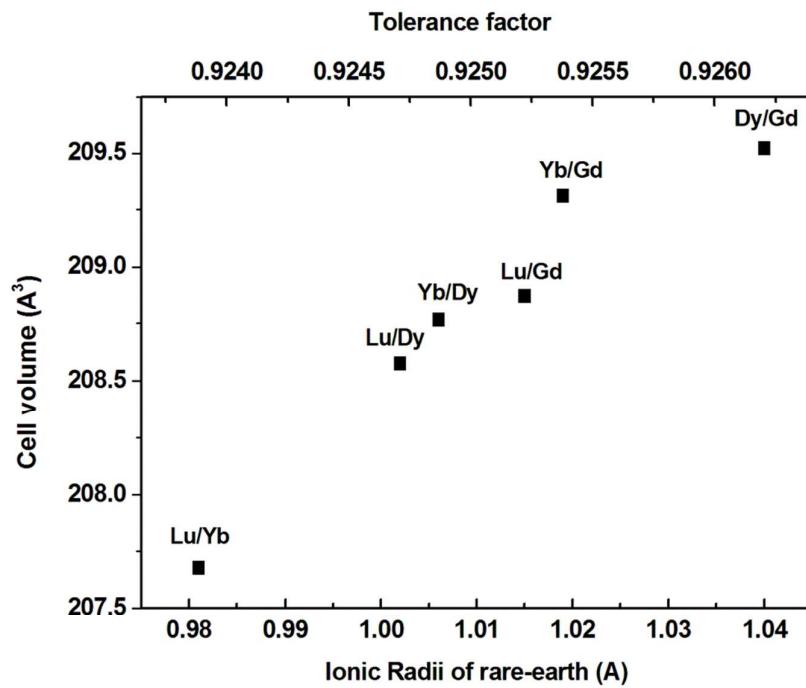


Figure S2. Unit cell volume (V) of $\text{Ca}_{0.9}\text{RE}'_{0.05}\text{RE}''_{0.05}\text{MnO}_3$ ($\text{RE}'/\text{RE}'' = \text{Yb/Lu, Dy/Lu, Dy/Yb, Gd/Lu, Gd/Yb, Gd/Dy}$) as a function of ionic radii of rare-earth ions and tolerance factor (t).

Figure S3

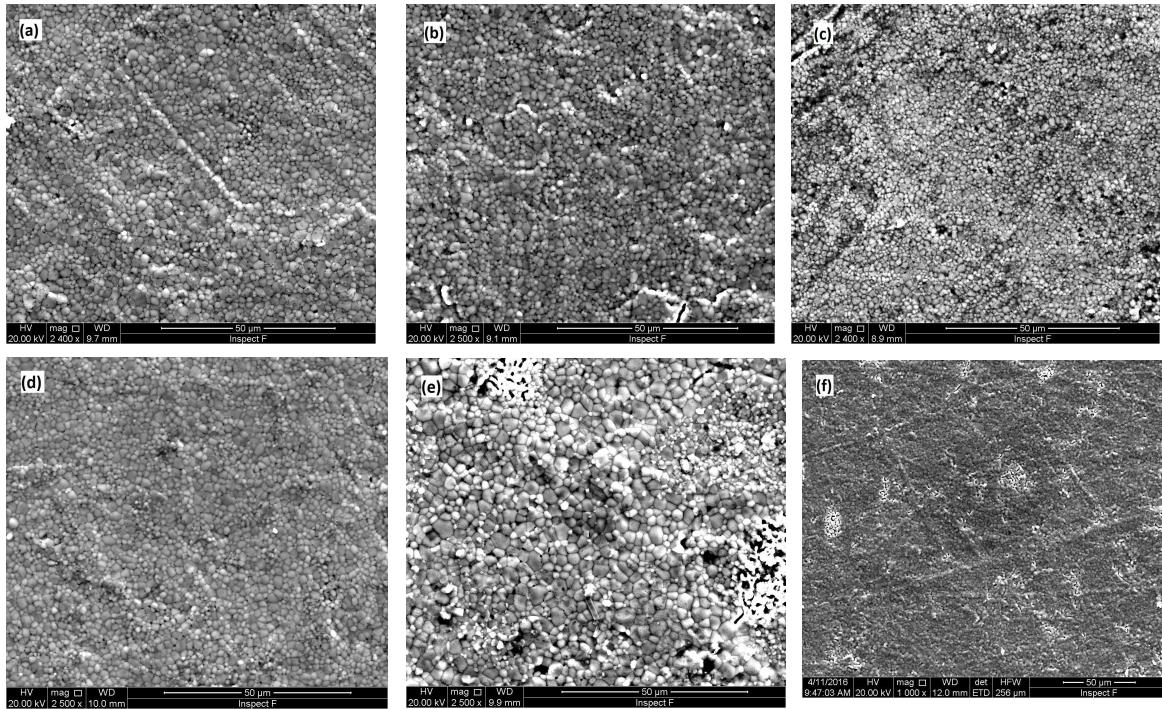


Figure S3. SEM micrographs showing sintered pellets under equivalent magnification: (a) $\text{Ca}_{0.95}\text{Dy}_{0.025}\text{Yb}_{0.025}\text{MnO}_3$, (b) $\text{Ca}_{0.95}\text{Gd}_{0.025}\text{Lu}_{0.025}\text{MnO}_3$, (c) $\text{Ca}_{0.9}\text{Dy}_{0.05}\text{Gd}_{0.05}\text{MnO}_3$, (d) $\text{Ca}_{0.9}\text{Dy}_{0.05}\text{Lu}_{0.05}\text{MnO}_3$, (e) $\text{Ca}_{0.9}\text{Gd}_{0.05}\text{Yb}_{0.05}\text{MnO}_3$ and (f) $\text{Ca}_{0.9}\text{Yb}_{0.05}\text{Lu}_{0.05}\text{MnO}_3$