Thermoelectric transport properties in metallic calcium aluminate, $Ca_{12}Al_{14}O_{33}$

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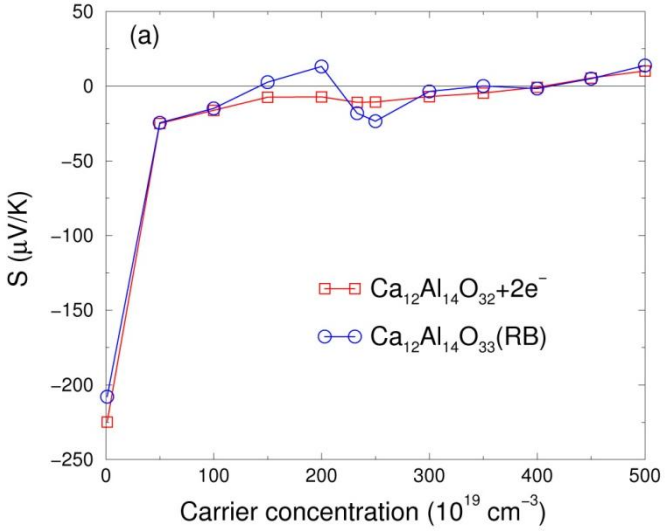
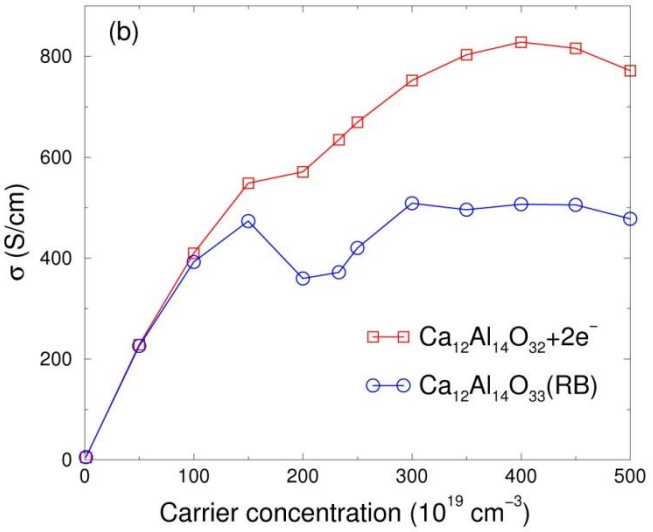
Structural, electronic, optical and thermoelectric properties of $Ca_{12}Al_{14}O_{33}$ and oxygen reduced $Ca_{12}Al_{14}O_{32}$+2e$^-$ have been calculated within first-principle density-functional approach. Our results for temperature- and carrier-dependent Seebeck coefficient and electrical conductivity, Figures (a) and (b), are in excellent agreement with experimental observations, Table.

Analysis of the calculated transport distribution reveals the origin of the observed change in the sign of thermopower – a reduced electron group velocity in specific directions of the Brillouin zone which appears due to unusual oxygen coordination of the Ca atoms.





Room-temperature electrical properties of oxygen reduced $Ca_{12}Al_{14}O_{33}$ obtained by Ca- and Ti-treatment for the specified number of days. The measured values are to be compared to the calculated values plotted on the right.

Sample	Conductivity S/cm	Thermopower μV/K
Ca - 4d	0.02	-280
Ca - 5d	3.7	-240
Ca - 10d	282.68	-7.86
Ti - 4d	1416	+6.97
Ti - 8d	1053	+4.6
Ti - 12d	567	-12.9