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Thermoelectric Properties and Band Structure Calculations of Novel Boron Network Compounds TAKAO MORI, TOSHIYUKI NISHIMURA, National Institute for Materials Science (NIMS), YURI GRIN, Max Planck Institute for Chemical Physics of Solids, TOETSU SHISHIDO, KAZUO NAKAJIMA, Institute for Materials Research, Tohoku University — Boron is an interesting element, tending to form atomic networks such as 2D atomic nets and clusters, with some analogy to carbon systems which have been more extensively studied. Boron has one less electron than carbon and thus is electron deficient when forming atomic networks, but this causes it to have a special affinity with the rare earth elements and as a result, many new compounds have recently been discovered [1]. Their potential as viable thermoelectric materials is attracting interest since they are high-temperature materials and possess intrinsic low thermal conductivity, with some compounds exhibiting Seebeck coefficients in excess of 200 μV/K above 1000 K. The thermoelectric properties and band structure calculations of novel borides such as $RB_{44}Si_2$, $RB_{17}CN$, $RB_{22}C_2N$, $RB_{28.5}C_4$ will be presented. Features in the band structure near the Fermi level indicate large doping effects in these compounds. Various doping experiments were carried out resulting in large increases to the figure of merit. [1] T. Mori, "Higher Borides," in: *Handbook on the Physics and Chemistry of Rare Earths*, Vol. 38, (North-Holland, Amsterdam, 2008) p. 105-173.

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