High throughput thermal conductivity of high temperature solid phases : the case of oxide and fluoride perovskites

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Phase transitions and anharmonicity at finite temperature deeply impact the value of thermal conductivity in perovskites and present a challenge for high-throughput studies. Using finite-temperature phonon calculations and machine-learning methods, we calculate the mechanical stability of about 400 semiconducting oxides and fluorides in the cubic perovskite form, at 0 K, 300 K and 1000 K. We find 92 mechanically stable compounds at high temperature – including 36 never mentioned in the literature previously – for which we calculate the thermal conductivity. We demonstrate that the thermal conductivity is generally smaller in fluorides than in oxides, due to a lower ionic charge, and describe simple structural descriptors that are correlated with its magnitude. Furthermore, we show that the thermal conductivity of most cubic perovskites decreases slower than the usual T^{-1} behavior. Finally, we also search for materials with negative thermal expansion and we describe a strategy to accelerate the discovery of mechanically stable compounds at high temperature.

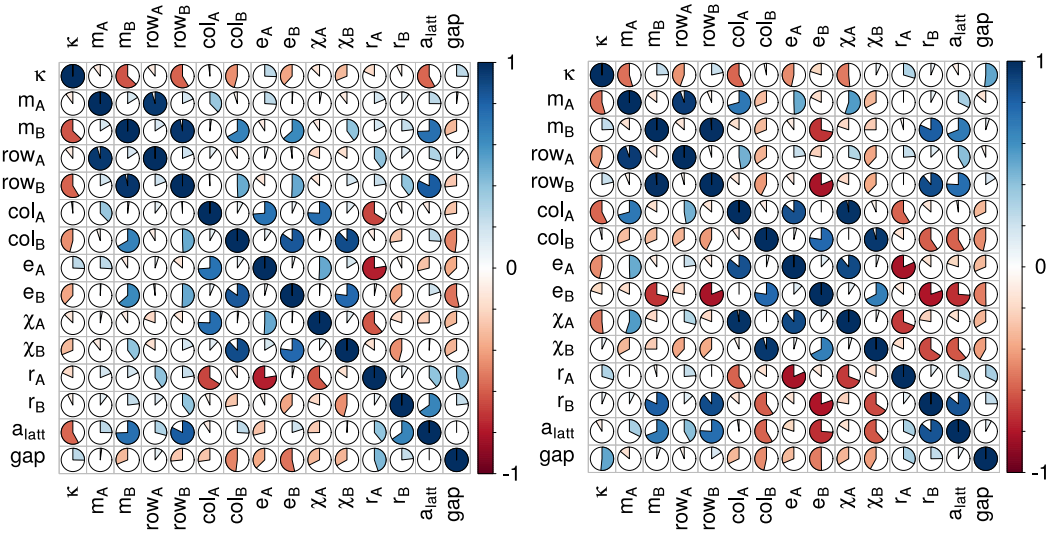

Fig. 1 – Correlograms between the thermal conductivity κ, the masses m_A and m_B of atoms at sites A and B of the perovskite ABX_3, their rows and columns in the periodic table row_A, row_B, col_A, col_B, their electronegativity e_A, e_B, their Pettifor scale χ_A, χ_B, their ionic radius r_A, r_B, the lattice parameter of the compound a_{latt} and its electronic gap, for mechanically stable fluorides (left) and oxides (right) at 1000 K.