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# Monte Carlo simulation of solid solutions in phases of petrological importance

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Recent research has shown that thermodynamic mixing properties of a binary solid solution (A,B)R can be predicted based on the excess static lattice energies of a few structures with the exchangeable atoms A and B arranged at specific positions within a supercell. The most important pairwise effective interactions (the energies of the exchange intra-crystalline reactions of AA + BB = 2AB type) can be extracted from the excess enthalpies of the structures with pairwise defects of AA and BB types inserted at all possible distances within the supercells of the end-members BR and AR. The limited number of these structures makes it possible to calculate the relevant enthalpies ab initio. The simulation of the temperature-dependent enthalpies of mixing can be performed with the Monte Carlo method based on the excess enthalpy defined as a function of the effective pair interactions and the frequencies of AB-type pairs. The free energies and the configurational entropies can then be evaluated with the help of the thermodynamic integration method. Examples of such calculations will be given for pyrope-grossular and stishovite-rutile solid solutions. The method will then be extended to cover coupled substitutions such as the solid solution of $MgSiO_3$-$Al_2O_3$ in perovskite.