Nampo4 triphylite and olivine phases

The shooter method is a modification of the shooter algorithm used in transition path sampling, which is employed here to systematically perturbate points in phase space [34]. The following general steps describe a typical shooter move simulation used throughout this body of work:

A small perturbation was applied to Na+ ions only, by setting a Gaussian half-width, centred on the velocity of each Na+ ions. An initial half-width was chosen in two different simulations regimes, as described below.

This process is repeated until the total simulation time reaches a target value of choice. Typical simulation times were in the order of 300-500 ps for mechanistic assessments and 3-5 ns for MSD/Diffusion Constants evaluations, as described below.

Normalised velocity autocorrelation function of Na+ ions within NaMPO4, (M = Mn left, M = Fe right) from MD simulation of an equilibrated structure at 700 K (red) and a resulting velocity distribution from a "Shooting" event (blue). The total simulation time was 10 ps, 10 vacf functions were calculated over 1 ps and averaged

The Gaussian half-width, which controls the extent of kinetic energy transfer between host framework and Na+ ions, was chosen within the interval [5.10-5-10-2 ?/fs], the limits corresponding to a low and high shooting regime, respectively. Most simulations (unless otherwise indicated) were performed using a longer delay of 2 ps between shooting events.

Self-diffusion coefficients were obtained from a shooting rate of 0.5 ps in order to maintain the separation in velocities between the Na+ ions and the framework. A narrower Gaussian half-width of 0.0001 ?2 fs-1 was used (Fig. A4).

Policies and ethics

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