SUPPORTING INFORMATION

Kinetic Monte Carlo simulations of ionic conductivity in oxygen ion conductors

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All simulations in the supporting information were performed for $Ce_{0.91}Sm_{0.09}O_{1.955}$ at 773 K with a lattice of 16×16×16 with the full model as stated in the main article.

Figure S1 shows the displacement of the oxygen ions parallel and perpendicular to the applied field in x-direction. The Gaussian form of the distribution in both cases originates from the self-diffusion of the oxygen ions. In x-direction an additional shift of the center can be observed due to the drift in the electric field. From this shift, the ionic conductivity can be calculated as described in the main article.

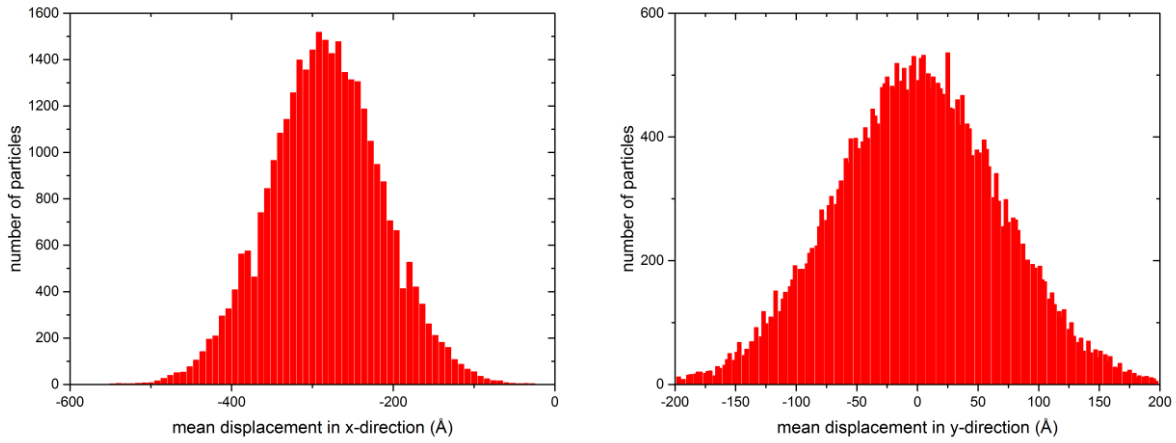

Figure S1: Displacement of the oxygen ions parallel (left) and perpendicular to the applied field.

Figure S2 shows the field dependence of the ionic conductivity averaged over ten simulations. Below approx. 0.2 $k_{\mathrm{B}}T$ the linear behavior is valid and the conductivity is independent of the field strength. Above this value the conductivity increases exponentially with the field strength. For values below 0.02 $k_{\mathrm{B}}T$ the statistical error increases due to the small induced drift of the ions.

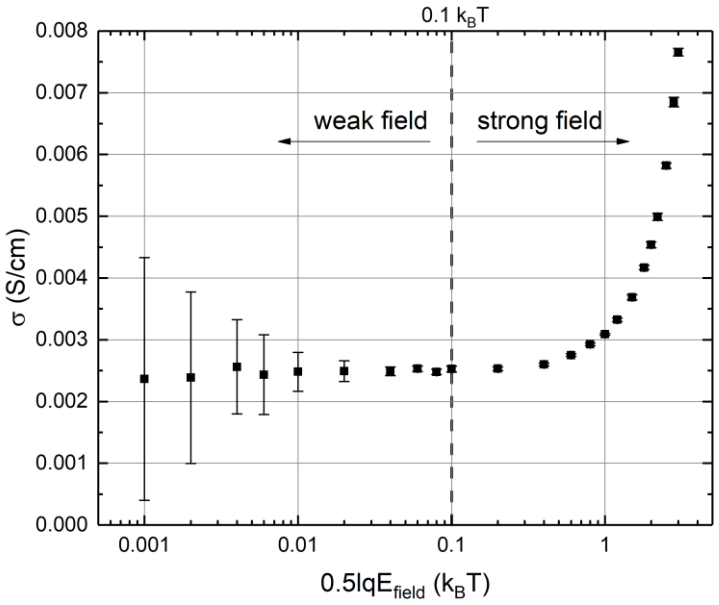

Figure S2: Simulated ionic conductivity as a function of the electric field strength E_{field}. *q* is the charge of the mobile ions and *l* is the jump distance. A field contribution of 1 $k_{\mathrm{B}}T$ equals an electric field strength of 2.46 MV cm^{-1}.

Figure S3 shows the mean displacement in direction of the electric field $\frac{\langle \vec{R} \cdot \vec{E} \rangle}{|\vec{E}|}$ depending on the simulated time. The mean displacement is a linear function of the simulated time.

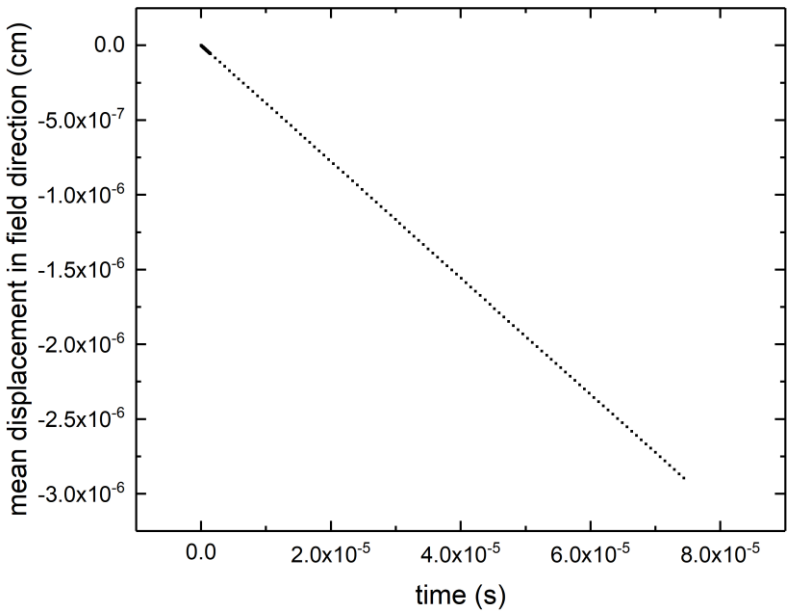

Figure S3: Mean displacement $\frac{\langle \vec{R} \cdot \vec{E} \rangle}{|\vec{E}|}$ of the mobile ions in direction of the electric field depending on the simulated time.