

Understanding the ionic conductivity maximum in doped ceria: trapping and blocking (Electronic Supplementary Information)

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I. SUPPLEMENTARY INFORMATION

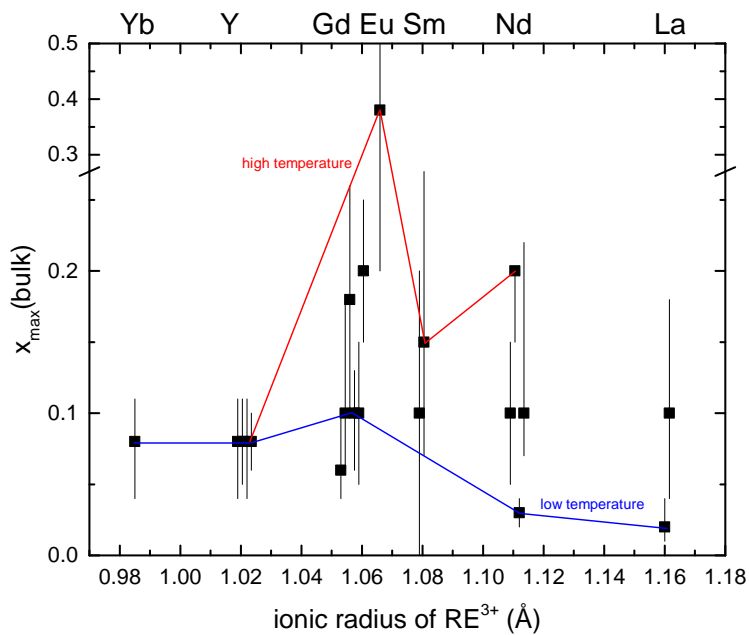


Figure S 1: Dopant fractions which lead to the highest bulk ionic conductivity for $\text{Ce}_{1-x_{\max}}\text{RE}_{x_{\max}}\text{O}_{2-x_{\max}/2}$ samples in the measured temperature range. Error bars show the nearest measured dopant fraction with lower conductivity. x_{\max} for low and high temperature measurements are marked.¹⁻¹¹

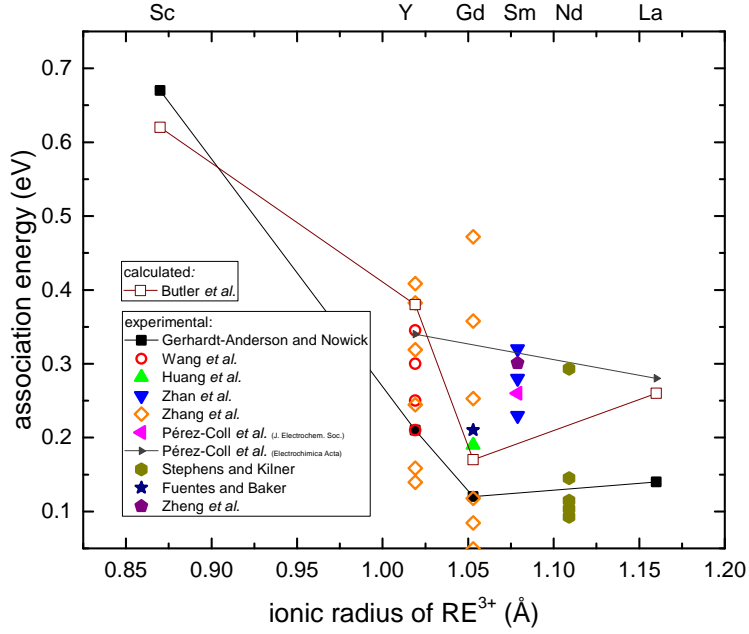


Figure S2: Association energies according to literature.^{3,9,12-21} Lines are a guide to the eye only.

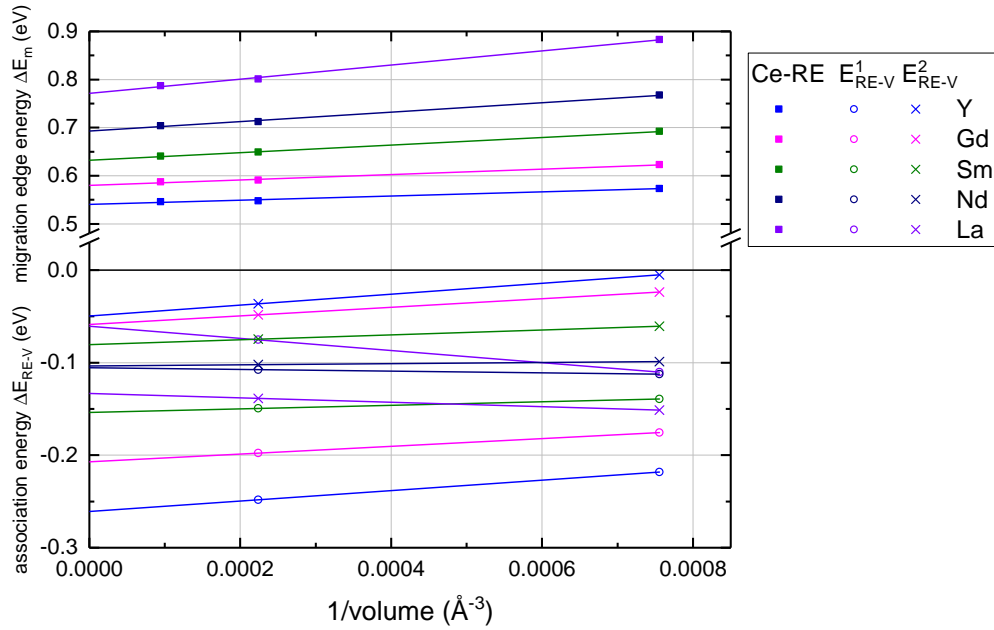


Figure S3: Migration energy of Ce-RE edge and RE-V interaction for different supercell sizes and $\Delta E^3_{RE-V} = 0$.

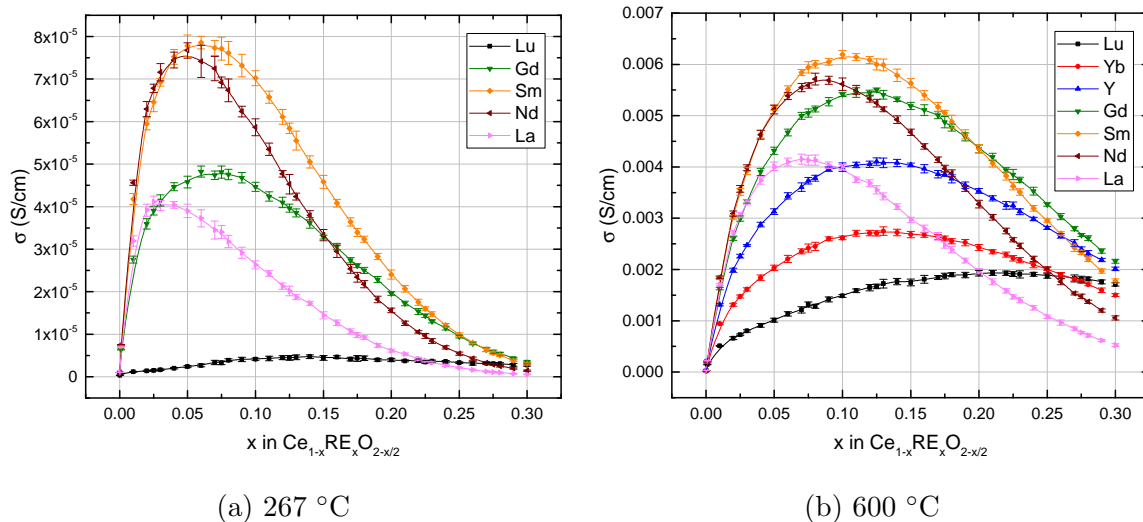


Figure S4: Ionic conductivity of rare-earth doped ceria at 267 °C and 600 °C with RE = Lu, Yb, Y, Gd, Sm, Nd and La calculated using KMC simulations. Lines are a guide to the eye only.

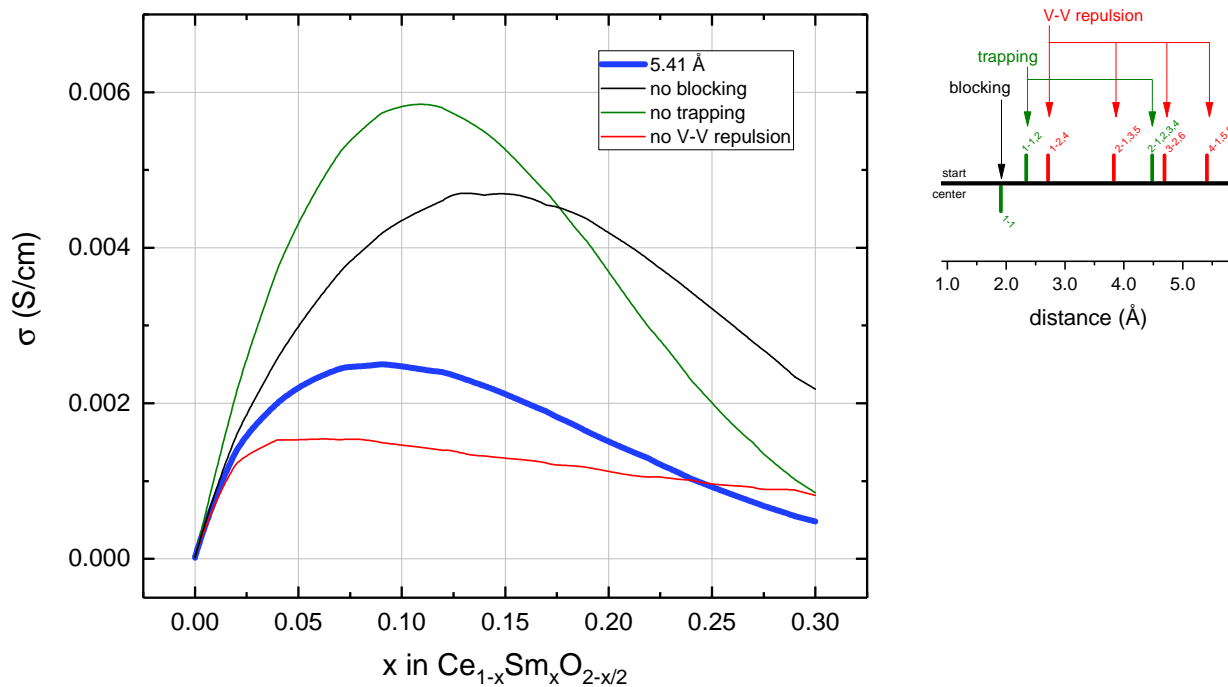


Figure S5: Simulated ionic conductivity of Sm doped ceria at 500 C (left) using blocking, trapping and V-V interactions with an interaction radius of 5.41 Å as shown on the right for the RE-V (green) and V-V interaction (red). Additionally, interactions are switched off individually.

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