

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

Julius Koettgen,¹ Steffen Grieshammer,^{1,2} Philipp Hein,¹ Benjamin
O. H. Grope,¹ Masanobu Nakayama,^{3,4} and Manfred Martin^{1,2,5,6}

¹*Institute of Physical Chemistry, RWTH Aachen University,
Landoltweg 2, 52056 Aachen, Germany*

²*Helmholtz-Institut Münster (IEK-12), Forschungszentrum Jülich GmbH,
Corrensstr. 46, 48149 Münster, Germany*

³*Frontier Research Institute for Materials Science (FRIMS),
Nagoya Institute of Technology, Gokiso,
Showa, Nagoya, Aichi 466-8555, Japan*

⁴*Center for Materials research by Information Integration (CM²),
Research and Services Division of Materials Data and Integrated System (MaDIS),
National Institute for Materials Science (NIMS),
1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan*

⁵*JARA-Energy, Forschungszentrum Jülich and RWTH Aachen University, Germany*

⁶*JARA-HPC, Forschungszentrum Jülich and RWTH Aachen University, Germany*

I. SUPPLEMENTARY INFORMATION

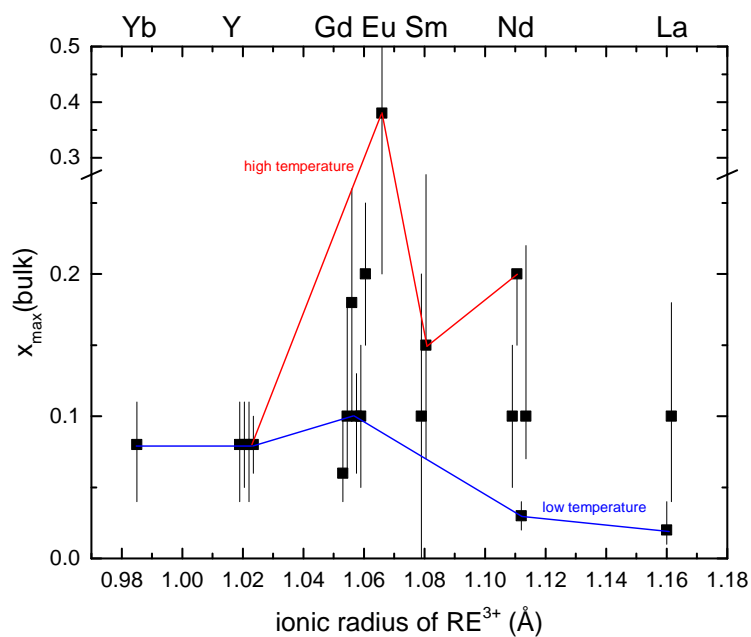


Figure S 1: Dopant fractions which lead to the highest bulk ionic conductivity for $\text{Ce}_{1-x_{\text{max}}}\text{RE}_{x_{\text{max}}}\text{O}_{2-x_{\text{max}}/2}$ samples in the measured temperature range. Error bars show the nearest measured dopant fraction with lower conductivity. x_{max} for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

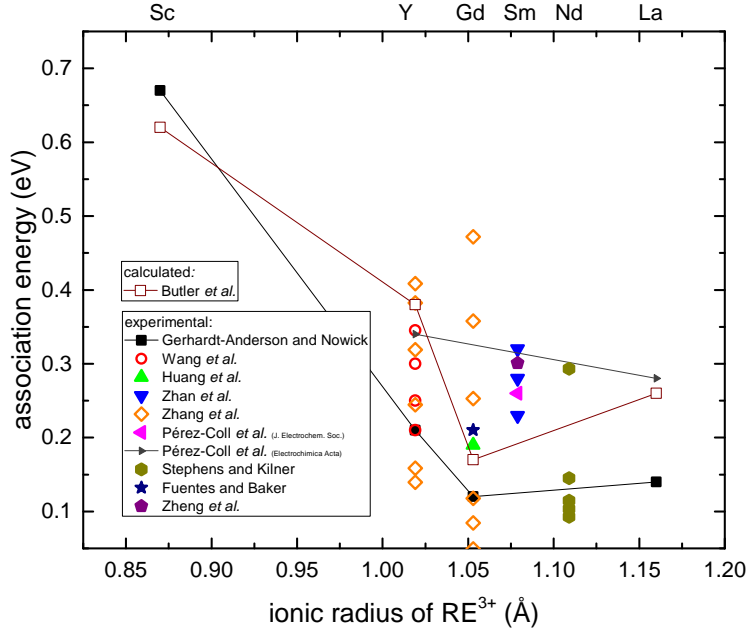


Figure S2: Association energies according to literature.^{3,9,12-21} Lines are a guide to the eye only.

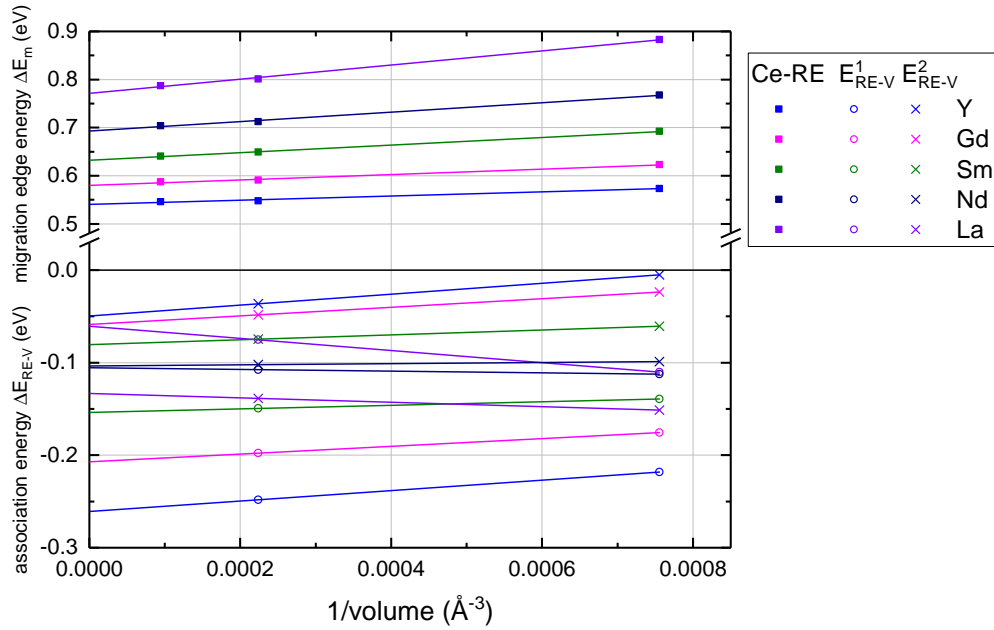


Figure S3: Migration energy of Ce-RE edge and RE-V interaction for different supercell sizes and $\Delta E^3_{RE-V} = 0$.

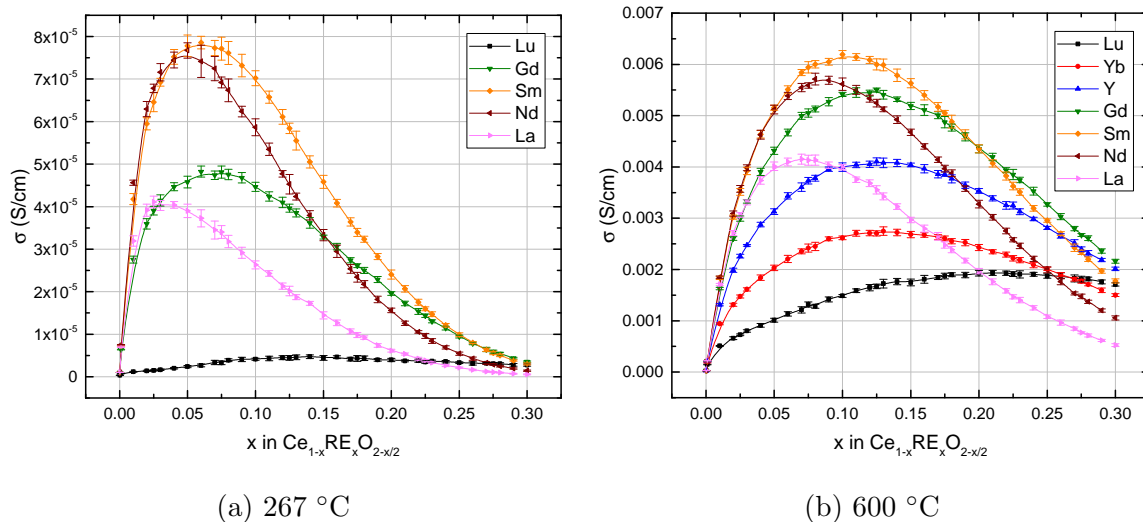


Figure S4: Ionic conductivity of rare-earth doped ceria at 267 °C and 600 °C with RE = Lu, Yb, Y, Gd, Sm, Nd and La calculated using KMC simulations. Lines are a guide to the eye only.

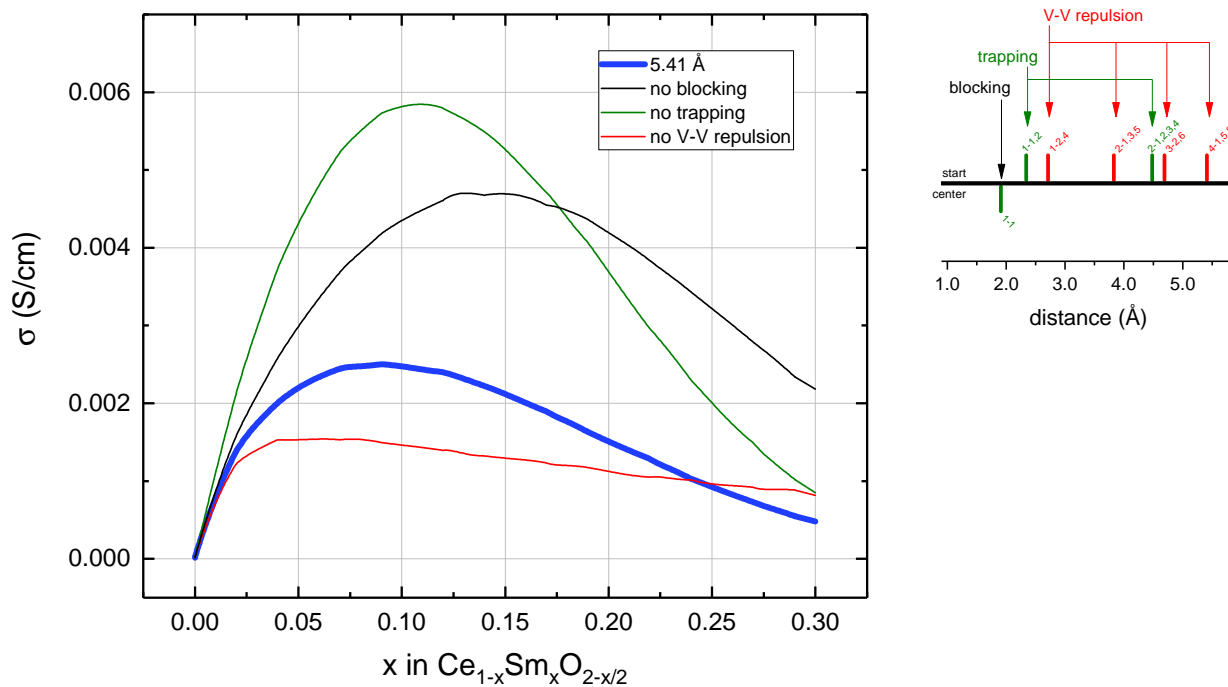


Figure S5: Simulated ionic conductivity of Sm doped ceria at 500 C (left) using blocking, trapping and V-V interactions with an interaction radius of 5.41 Å as shown on the right for the RE-V (green) and V-V interaction (red). Additionally, interactions are switched off individually.

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