Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Electronic Supplementary Information for

New Interatomic Potential Parameters for Molecular Dynamics Simulations of Rare-Earth (RE = La, Y, Lu, Sc) Aluminosilicate Glass Structures: Exploration of RE^{3+} Field-Strength Effects

Kirill Okhotnikov, Baltzar Stevensson and Mattias Edén*

Physical Chemistry Division, Department of Materials and Environmental Chemistry, Arrhenius Laboratory, Stockholm University, SE-106 91 Stockholm, Sweden

*Corresponding author. E-mail: *mattias.eden@mmk.su.se*

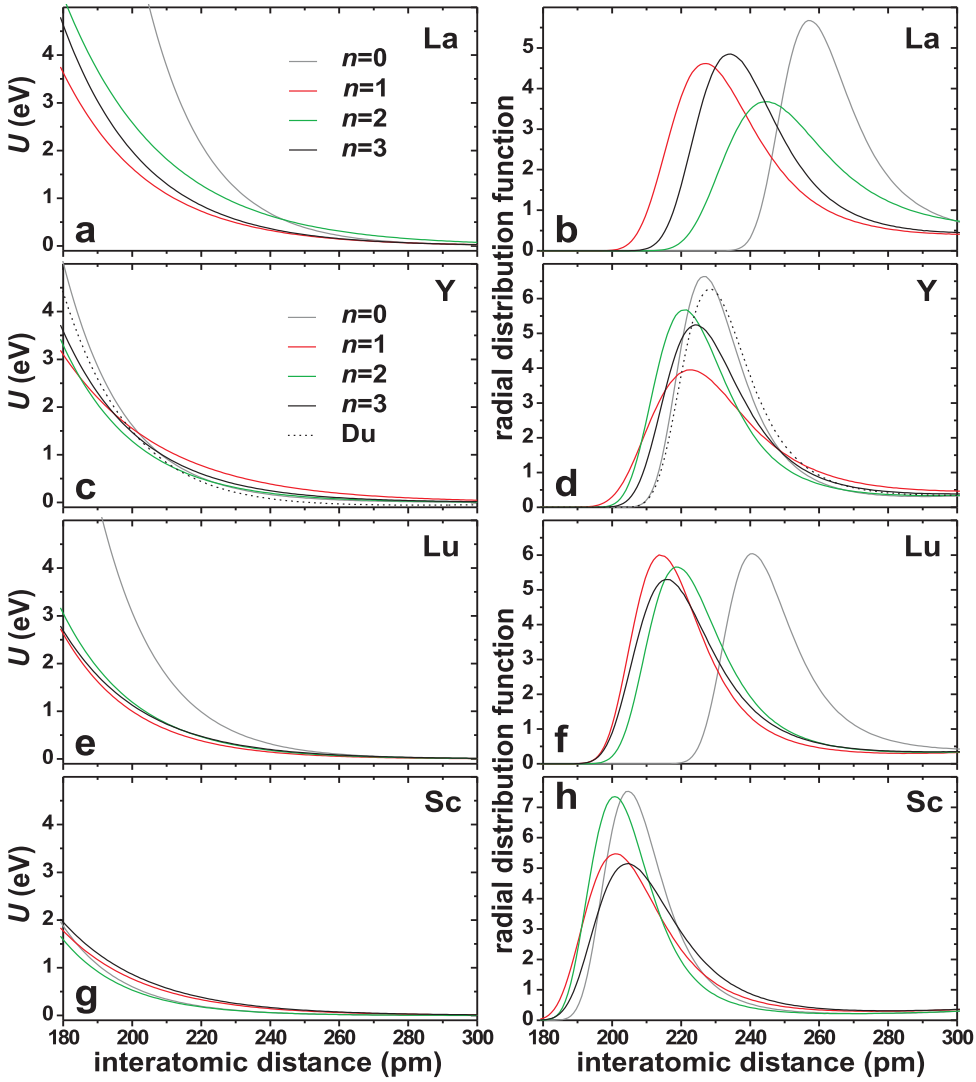

Figure S1. Potential energies (left panel) evaluated from Eq. (4) of the main text, and RDFs (right panel), both plotted for increasing RE–O distance and calculated for the RE(2.21) glass compositions. The parameters $S^{(n)} \equiv \{A^{(n)}_{\text{RE–O}}, \rho^{(n)}_{\text{RE–O}}\}$ are associated with increasing degrees of iteration ($0 \leq n \leq 3$) and were employed for RE corresponding to (a, b) La; (c, d) Y; (e, f) Lu, and (g, h) Sc. (a) identifies each curve with its respective set $S^{(n)}$. (c, d) also display the results of instead using the Y–O interionic potential of [J. Du, *J. Am. Ceram. Soc.*, 2009, **92**, 87-95] *via* Eq. (3) of the main text. The values $\{A^{(3)}_{\text{RE–O}}, \rho^{(3)}_{\text{RE–O}}\}$ of the last iteration stage are listed in Table 1 and were used in all other evaluations/simulations.