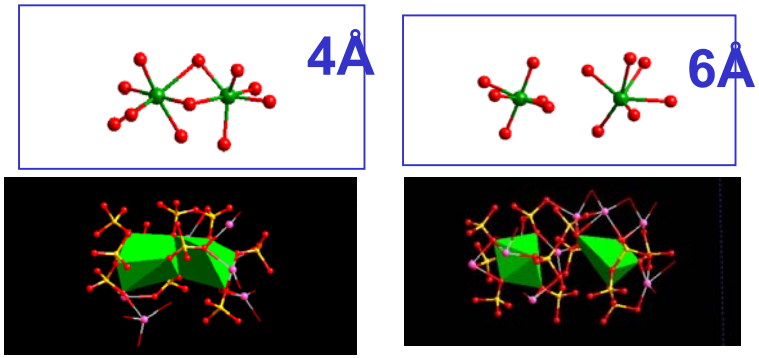
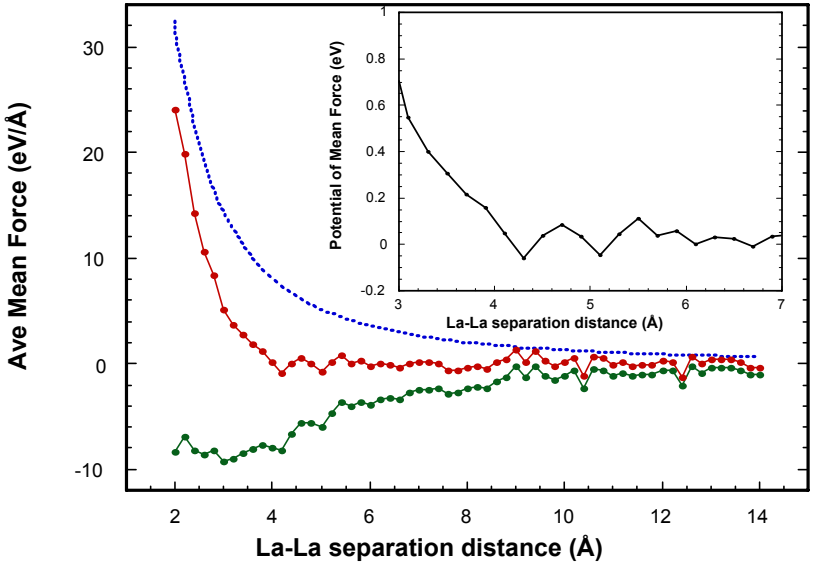
Pilot-EMSLJ2 Highlight

EMSL

Driving Force of Lanthanide Clustering in Silicate Glass

L. René Corrales and Byeongwon Park





- **The use of liquid state theory reveals the solvent shell-like structure of a glass network about the La cations.**
- **The calculated mean force (and potential of mean force) of an ion pair along a reaction coordinate suggests that the network drives the aggregation of the La cations via a cavity coalescence mechanism**
- **The barriers in the PMF reveal that an oxygen ion is stripped from the network to form free oxygen anions in the form of La-O-La bridges.**

B. Park, H. Li, L. R. Corrales, "Molecular dynamics simulation of La_2O_3-Na_2O-SiO_2 glasses: I. The structural role of La^{3+} cations", J. Non-Cryst. Solids (in press).

The mean force (red curve) is determined from molecular dynamics (MD) simulations. The direct force (blue curve) is the bare ion Coulomb force. The solvent force (green curve) is the difference of the mean and direct forces. The inset shows the potential of mean force (PMF), determined by integrating the mean force. The data is an average of four independent MD simulations.