Applying Non Equilibrium and Constrained Molecular Dynamics to the Soret Effect in Solids with Charged Defects

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Thermal diffusion has been studied mostly in fluids, notably for the oil industry, experimentally and also theoretically. Among solids, oxides composing nuclear fuels can be submitted to a significant oxygen transport by this mechanism. The rare experimental studies have been found to be difficult; Molecular Dynamics techniques are expected to help characterize this phenomenon. Uranium oxide UO2+x presents two specificities: the oxygen pressure varies considerably with its oxygen composition it shows localized electronic defects that are challenging to model by classical atomistic techniques. We will present the different techniques consistent with this specificities in order to evaluate the heat of transport as a function of the oxygen composition.