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## Atomic scale calculations of thermophysical properties of molten salt reactor fuel via DFT and PIM MD simulations: inclusion of Americium.

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In recent years, interest in molten salt reactors has been growing due to their intrinsic safety, facilitation of certain operation and management tasks and their potential for actinide conversion. In this research field, a highly important aspect for determining design parameters is knowing as accurately as possible the properties of the fuel itself (density, heat capacity, viscosity, conductivity, thermal expansion, etc.). However, due to challenging conditions encountered in experiments, such as corrosion, high temperatures, and, specifically in the case of actinides, radioactivity, numerical determination of these properties appears important and necessary for this purpose.

To study salt mixtures based on actinide chlorides like NaCl-PuCl<sub>3</sub>, NaCl-(Pu/Am)Cl<sub>3</sub>, and NaCl-MgCl<sub>2</sub>-(Pu/AmCl<sub>3</sub>), atomic-scale simulation techniques such as Molecular Dynamics (MD) are employed. To effectively calculate the properties, it is necessary to use a type of interatomic potential suitable for ionic melts, such as the so-called PIM potential <sup>[1]</sup>, whose parameters can be fitted using force-matching methods based on Density Functional Theory (DFT) results. With this method, the parametrisation of the interatomic potential is done minimising the error between the reference DFT forces and the ones predicted from the PIM model.

The strategies and techniques used to include americium to the PIM potential are presented in this work. This is carried out in order to investigate actinide chlorides XCl<sub>3</sub> (X=U, Pu, and Am) /NaCl binary systems. Moreover, a comparison between available experimental results and simulations of chosen parameters for DFT simulations using the CP2K code <sup>[2]</sup> (PW cut-off, basis set etc.) are shown, in addition to preliminary MD results on binary systems.

[1] (Salanne & Madden, 2011-10-10)

[2] (Kühne, 2020-05-21)