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# Atomic scale calculation 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. More in detail, this technology would be able to increase the technology capability of Americium and other minor actinides conversion. In this research field, a highly important aspect for determining design parameters knows as accurately as possible the properties of the fuel itself (density, heat capacity, viscosity, conductivity, expansion, etc.). In MSR, still, this need is even more accentuated due the strong correlation between neutronics, thermo-hydraulics and chemistry. The principal cause of these features is the liquid phase of the fuel, a different concept compared to the most traditional actinides oxides. 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. This technique permits to compute crucial properties of the material thanks to statistical mechanics formalism. Yet, 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. Moreover, it is important to not forget the difficulties encountered when dealing with actinides at atomic scale. This is due to mainly to their complex electronic structure that requires complex modelling procedures. 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 plus the 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.

## References

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- [2] T. Kühne et al., *The Journal of Chemical Physics* **152**, 194103 (2020).