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## Atomic scale calculations of thermophysical properties of Americium-based molten salt for next generation nuclear reactors.

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Due to their intrinsic safety, capability to convert minor actinides, homogeneity of the fuel and low pressure required, molten salt reactors (MSRs) have known a renewed interest over the last few years. Moreover, they represent an innovative and effective possible solution to fulfil the French objective of closure of fuel cycle. Pu produced in the current PWR fleet can be used to do fission and eventually to produce energy but also the minor actinides can be transmuted. In fact, minor actinides such as Americium could be converted in elements with lower radioactivity and half-life. Yet, to fulfil this purpose a fast neutron spectrum must be used, which is possible in MSRs, unlike for example in PWRs.

Still, their development remains hampered down by crucial scientific and technological challenges, especially concerning the system dimensioning and fuel behaviour under irradiation and/or corrosion. Indeed, to determine design parameters we need to know as accurately as possible the properties of the fuel itself (density, heat capacity, viscosity, conductivity, expansion, etc.) due to the strong correlation between neutronic, thermo-hydraulics and chemistry, and given the liquid phase of the fuel.

However, due to the challenging conditions encountered in experiments, such as corrosion, high temperatures, and, specifically in the case of actinides, radioactivity, performing numerical computations of these properties in order to complete the experimental datasets appears to be a necessary alternative.

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>), simulation techniques such as classical Molecular Dynamics (CMD) 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. Yet, to do so, the DFT setup must be tested and give reasonable and numerically stable results, a difficult task when dealing with minor actinides for example, due to their complex electronic structure. Moreover, an additional challenge comes from the difficulty to have experimental data for the validation.

In this work, consequently, our target is to find a suitable DFT setup to parametrise the interatomic potentials that must include elements such as Americium or Plutonium. In addition, we leverage CMD to compute the thermophysical properties cited above. In addition, a validation of our models by simulating and comparing our results to Raman spectra will be performed.

The strategies and techniques used to include americium to the PIM potential will be presented in this work such as the inclusion or not of dispersion corrections. Moreover, we will show results concerning binary salts and our strategies to simulate Raman spectra to validate our approach.

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

[2] (Kühne, 2020-05-21)