

Molten salt thermo-physical property prediction using machine learning interatomic potentials

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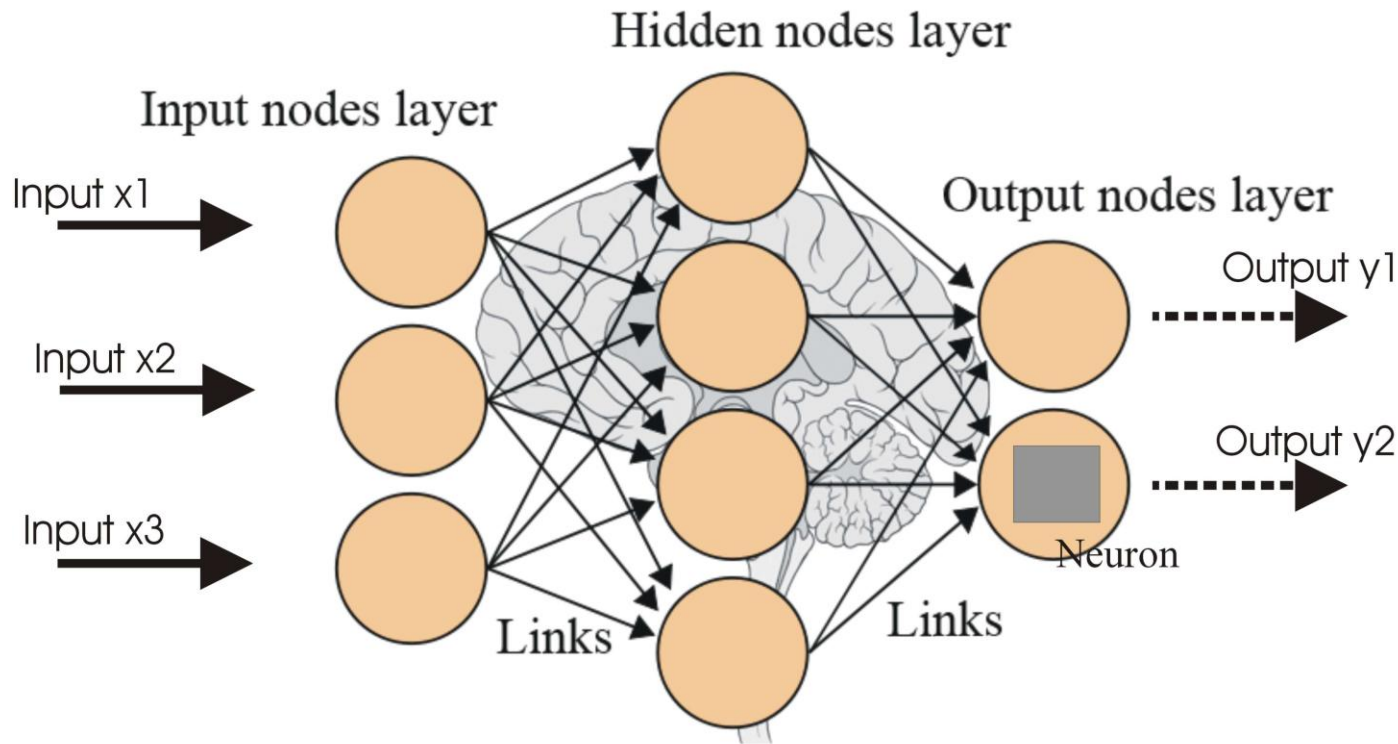
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Background

- $\text{LiF-BeF}_2\text{-UF}_4$ mixtures have been historically used as fuel salts in molten salt reactors, where Li_2BeF_4 (FLiBe) base acts as solvent for fissile UF_4 (~0.5-2 mol%).
- Accurate knowledge of the thermo-physical properties of molten salts is essential for the design and safety of molten salt reactors. For example, thermal expansion of fuel salts (reduced density) can increase neutron leakage, reducing fission rate.
- Due to their corrosive and radioactive nature, experimental measurements of the thermo-physical properties of $\text{LiF-BeF}_2\text{-UF}_4$ salts are challenging and limited (mostly from Mound Laboratory in the 1950s).
- With the advent of AI/ML, thermo-physical properties of molten salts can be predicted with good accuracy using molecular dynamics (MD) simulations driven by neural network-based machine learning interatomic potentials (NNPs).
- Computer generated molten salt data over a wide composition and temperature range can be used to bridge experimental knowledge gaps and populate molten salt property databases such as MSTDB-TP.



Quick introduction to neural networks



A neural network can approximate any continuous function arbitrarily well.

– Universal Approximation Theorem

Let f be any continuous function on a compact subset of $\mathbb{R}^n$.
Then for any $\varepsilon > 0$, there exists a feedforward neural network with

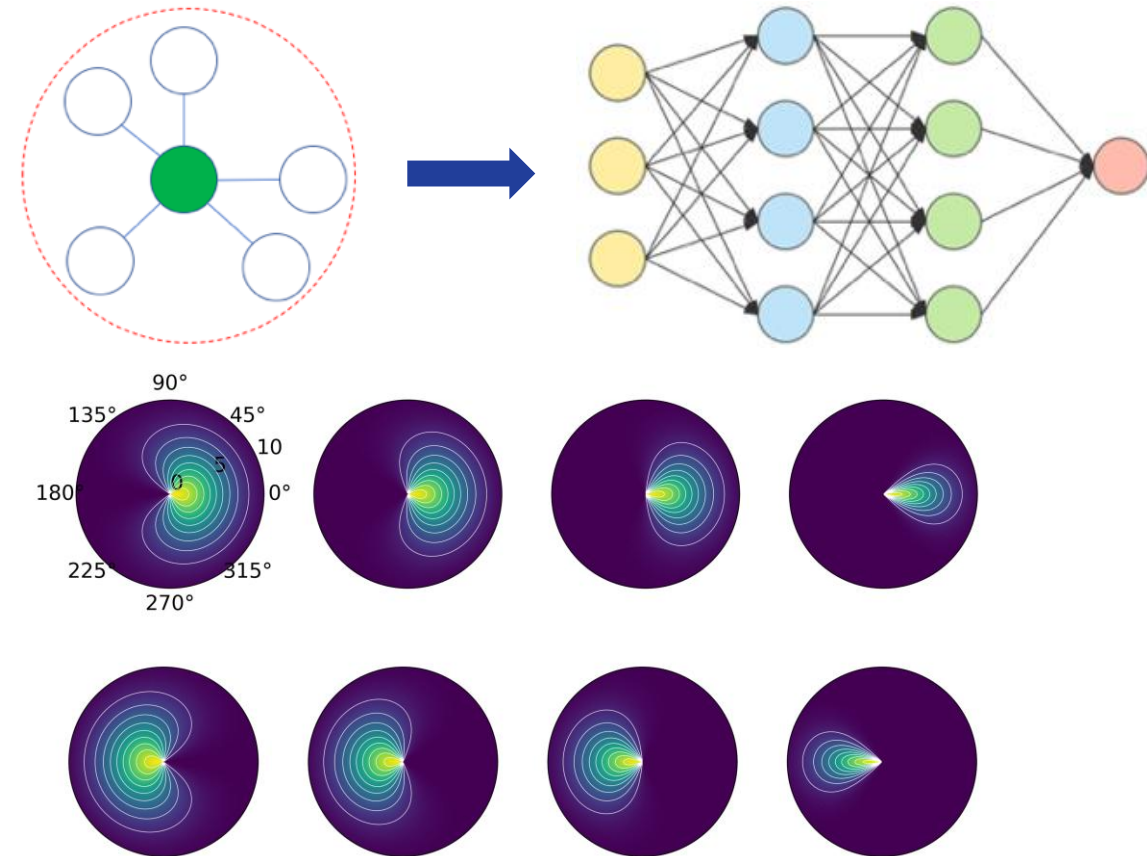
- "one hidden layer,"
- "a finite number of neurons,"
- "and a suitable non-linear activation function such that the network g satisfies"

$$\sup_x |f(x) - g(x)| < \varepsilon.$$



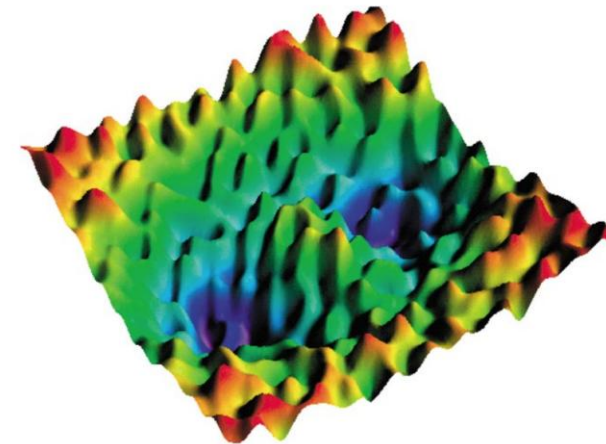
Why NNP?

$$E_{total} = \sum_i E_i$$



Because neural network potentials (NNPs) are not restricted to predefined functional forms, they can accurately reproduce complex DFT potential energy surfaces far better than empirical potentials.

NNPs are also orders of magnitude faster than DFT, enabling large-scale MD simulations.



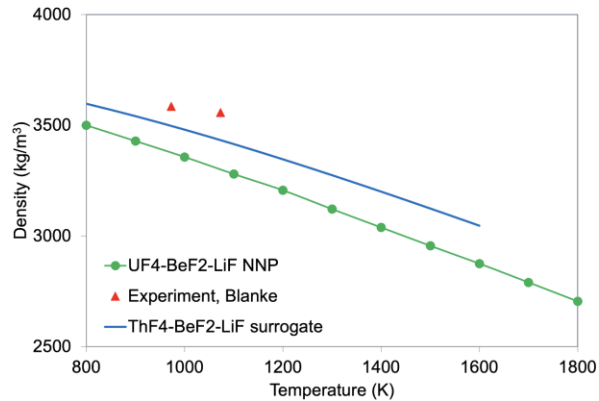
Why developing NNP for LiF-BeF₂-UF₄ is challenging

- U⁴⁺ ions (electron configuration [Rn]5f²) exhibit local magnetic moments due to two unpaired 5f electrons.
- Spin-polarized DFT calculations for U⁴⁺-containing salts can converge to different spin and orbital configurations depending on initial settings such as magnetic moments.
- This introduces small noise in DFT energies and forces, which can be inadvertently learned by machine-learning models such as NNPs, degrading their performance in MD simulations.
- In paramagnetic UF₄-containing salts, the local moments on U⁴⁺ ions are dynamically fluctuating and thermally disordered. This randomness is difficult to model within a single, deterministic DFT framework.
- In this study, LiF-BeF₂-ThF₄ is introduced as an f-electron-free surrogate for LiF-BeF₂-UF₄. The absence of f-electrons and local magnetic moments in Th⁴⁺ ions (electron configuration [Rn]) leads to stable and consistent DFT training data.

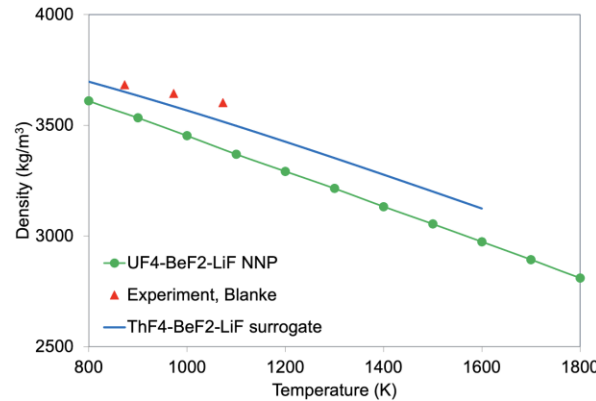


NNP-predicted properties for $\text{LiF-BeF}_2\text{-UF}_4$ salts

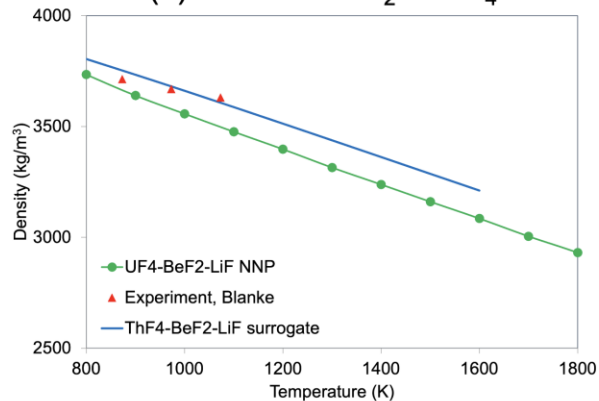
Density



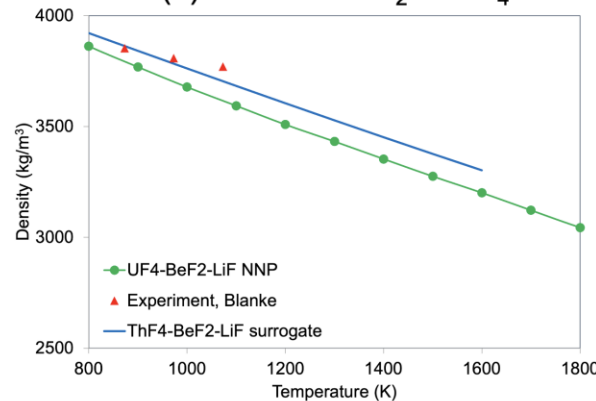
(a) 40LiF-40BeF₂-20UF₄



(b) 50LiF-30BeF₂-20UF₄

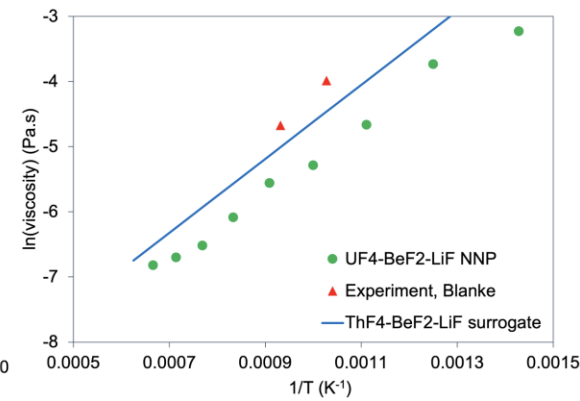


(c) 60LiF-20BeF₂-20UF₄

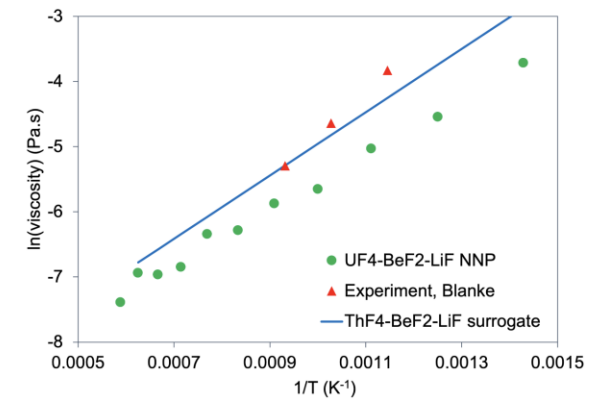


(d) 70LiF-10BeF₂-20UF₄

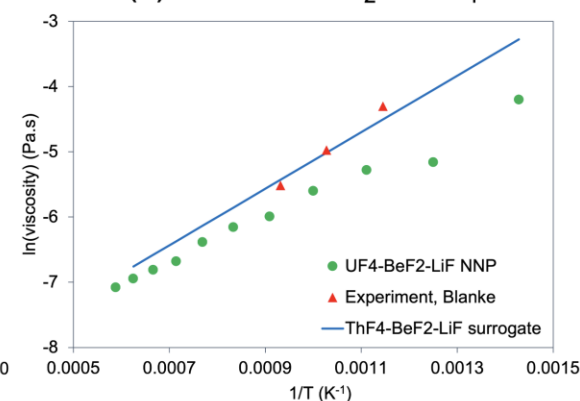
Viscosity



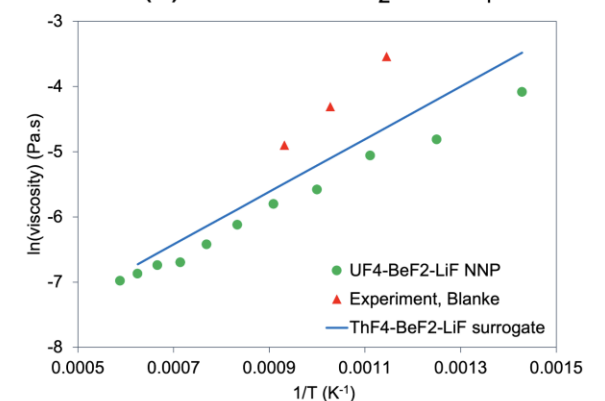
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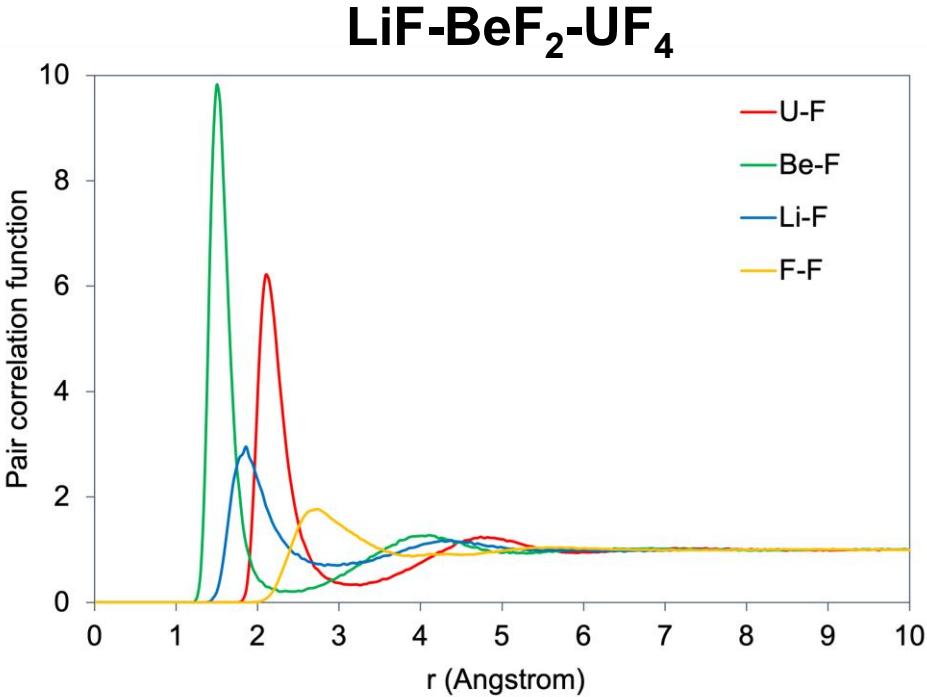


(d) 70LiF-10BeF₂-20UF₄

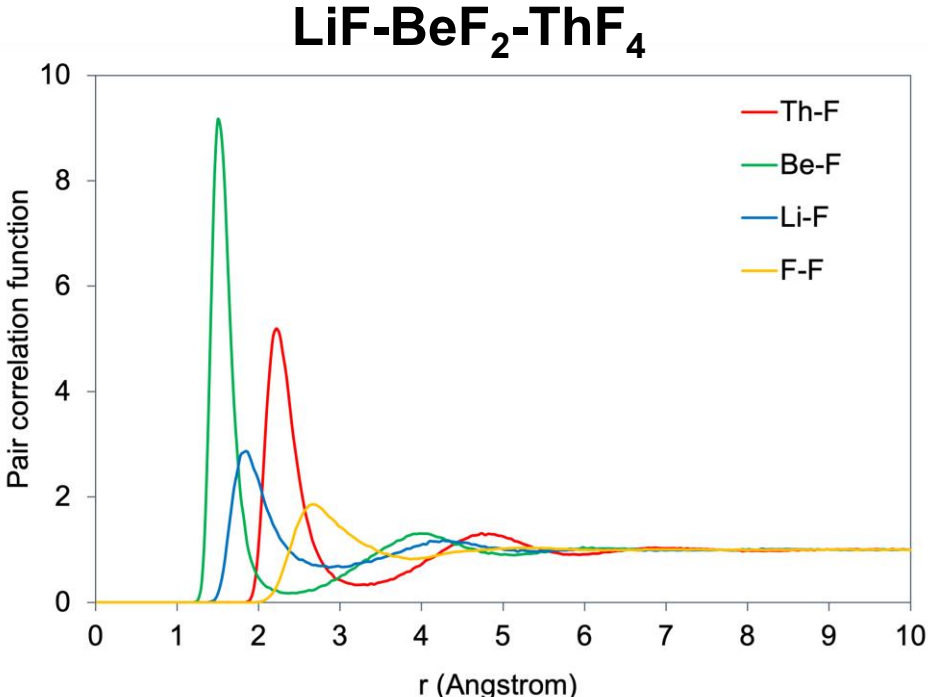


Structures of $\text{LiF-BeF}_2\text{-UF}_4$ and $\text{LiF-BeF}_2\text{-ThF}_4$ salts

PCF



Pair	NNP
Be-F	1.50
U-F	2.10
Li-F	1.86



Pair	NNP	AIMD
Be-F	1.50	1.54
Th-F	2.22	2.26
Li-F	1.86	1.84

Bond length

Summary

- Machine-learning interatomic potentials, such as neural network potentials, can accurately capture the complex potential energy surfaces of multi-component molten salt systems.
- These ML potentials enable high-temperature molecular dynamics simulations that serve as cost-effective alternatives to challenging experimental measurements.
- ML-driven predictions of thermophysical properties across wide temperature and composition ranges help bridge critical data gaps in molten-salt reactor design and support population of databases such as MSTDB-TP.
- UF_4 -based molten salts present unique challenges due to their complex electronic and magnetic behavior associated with the two 5f electrons of U^{4+} , which can introduce noise and non-uniqueness in DFT training data and impact the stability and accuracy of ML models.
- This work demonstrates the effectiveness of $\text{LiF-BeF}_2\text{-ThF}_4$ as a surrogate system for modeling the thermo-physical properties of $\text{LiF-BeF}_2\text{-UF}_4$ salts.



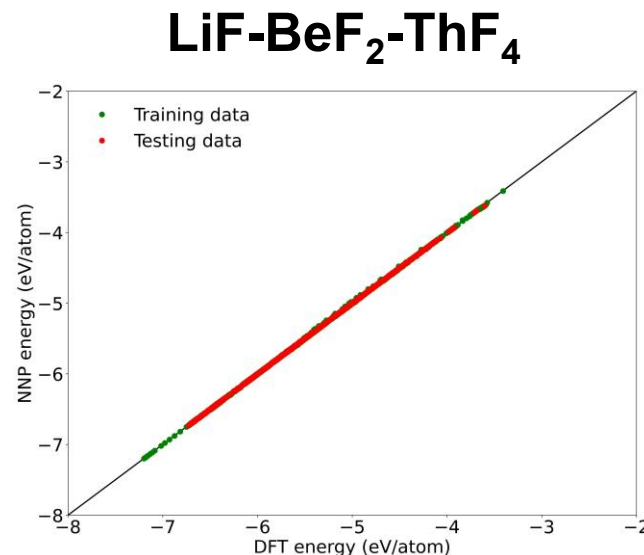
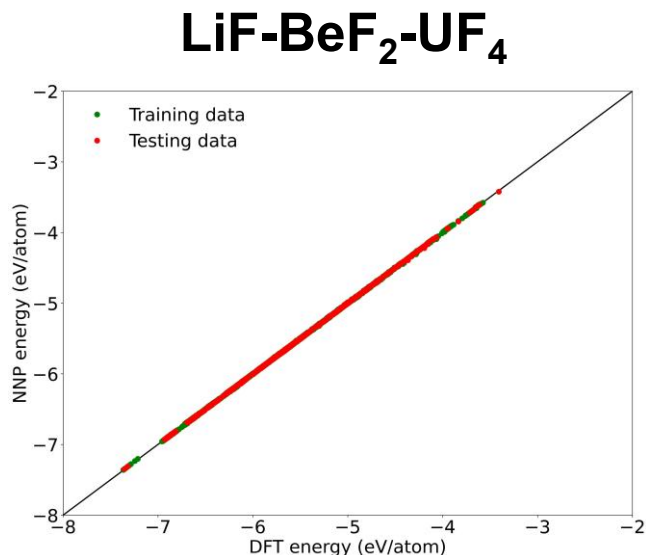


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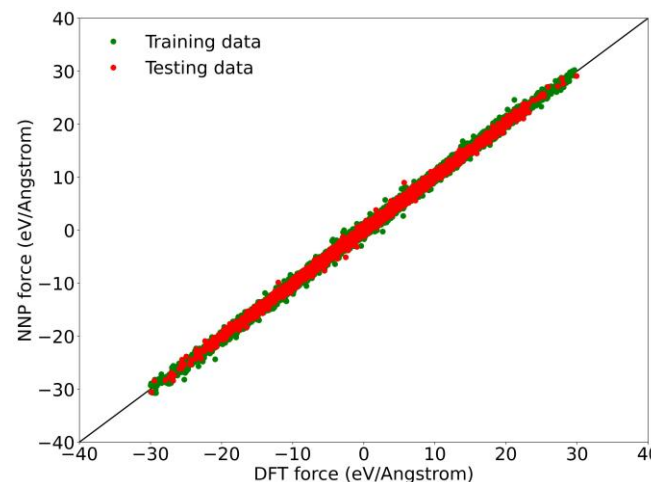
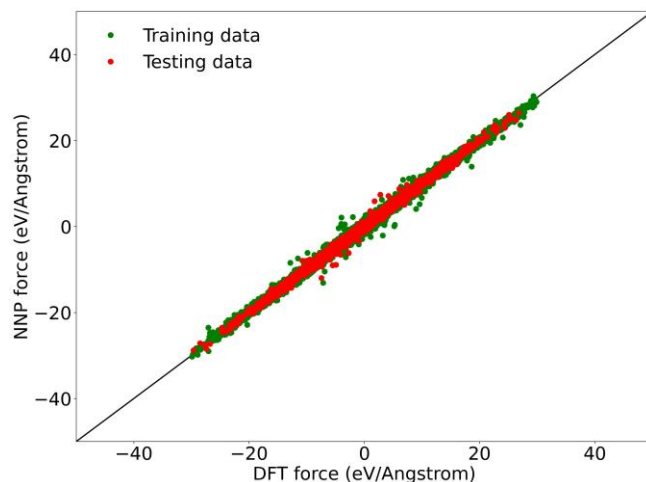
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NNPs for $\text{LiF-BeF}_2\text{-UF}_4$ and $\text{LiF-BeF}_2\text{-ThF}_4$ salts

Energy



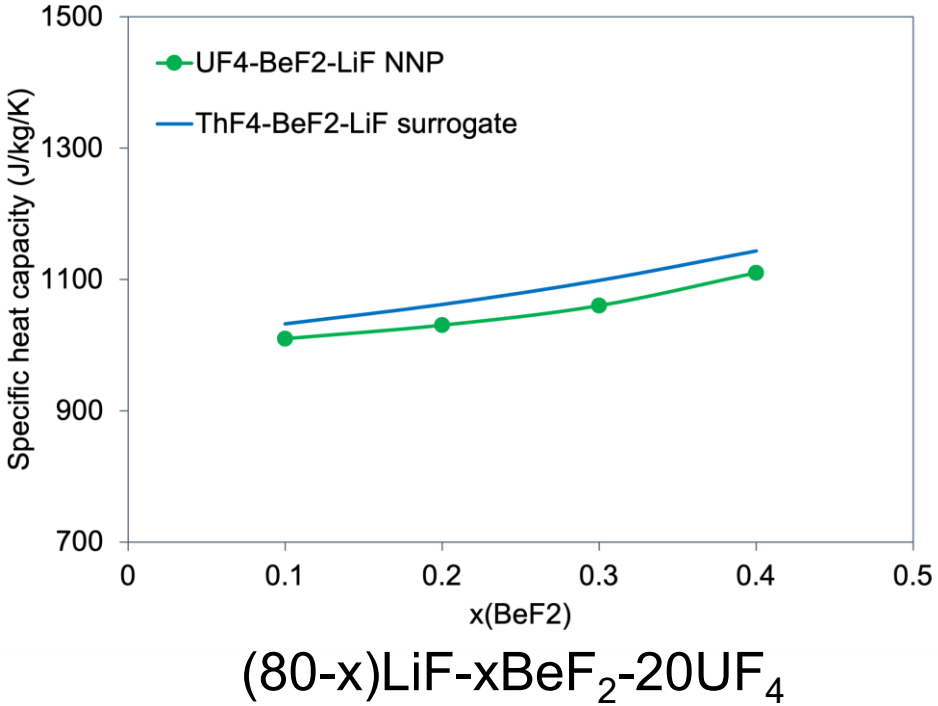
Force



- In this work, a ferromagnetic (FM) approximation was adopted to model $\text{LiF-BeF}_2\text{-UF}_4$ salts.
- While this approach captures the presence of unpaired electrons, it introduces an unphysical long-range magnetic ordering in the liquid state, which is absent in real melts.
- This difficulty does not arise for $\text{LiF-BeF}_2\text{-ThF}_4$, which is intrinsically nonmagnetic.



Specific heat capacities of LiF-BeF₂-UF₄ salts



System	Density	Heat capacity	Viscosity	Thermal conductivity
LiF-BeF ₂ -UF ₄	36	0	38	2
LiF-BeF ₂ -ThF ₄	3	0	2	0