A Bayesian Methodology for Constructing Ternary Phase Diagrams: The LiF–NaF–KF System

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This work presents a Bayesian methodology [1] for constructing phase diagrams of salt systems, applied to the ternary LiF–NaF–KF system. The approach combines Gaussian process regression with molecular dynamics data that include statistical uncertainties. Molecular dynamics are performed using a Moment Tensor Potential [2,3], parametrized via active learning on density functional theory calculations. The Gibbs free energy surfaces are reconstructed from their temperature and composition derivatives using Gaussian process regression, and the phase diagrams are obtained via the common tangent method.
The methodology was validated on the binary NaF–KF system and successfully applied to the ternary LiF–NaF–KF system, with both diagrams showing good agreement with experimental data. Computational costs were below 20,000 CPU hours for the binary diagram and approximately 100,000 CPU hours for the ternary diagram, demonstrating the scalability and practical applicability of the approach.

[1] Miryashkin T, Klimanova O, Ladygin V and Shapeev A 2023 *Physical review. B, Condensed matter* **108** 174103
[2] Shapeev A V 2016 *Multiscale Modeling & Simulation* **14** 1153–1173
[3] Novikov I S, Gubaev K, Podryabinkin E V and Shapeev A V 2020 *Machine Learning: Science and Technology* **2** 025002