Resolving the In–Au–Hg phase diagram using Bayesian learning

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This work investigates In-Au-Hg amalgams for applications in mercury gas-discharge lamps. Temperature-composition phase diagrams are constructed to identify amalgam compositions with elevated melting temperatures, enabling higher lamp performance.
Gaussian process regression is applied to molecular dynamics (MD) simulation data with quantified statistical uncertainties, allowing the reconstruction of Gibbs free energies as functions of temperature and composition. MD simulations are performed using the Moment Tensor Potential (MTP) [1]. The developed methodology yields phase transition boundaries with associated confidence intervals in the thermodynamic limit for both binary [2] and ternary systems. The approach is applied to the construction of the In–$Au_{0-0.33}$, In–$Hg_{0-0.2}$, and In–$Au_{0-0.33}$–$Hg_{0-0.2}$ phase diagrams.
The resulting phase diagrams show good agreement with available experimental data [3–5], up to a systematic temperature shift attributable to the accuracy of the DFT calculations used for MTP training.

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