Abstract Submitted
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Solid-liquid phase coexistence of alkali nitrates from molecular dynamics simulations SAIVENKATARAMAN JAYARAMAN, Sandia National Laboratories, EDWARD MAGINN, University of Notre Dame, ANATOLE LILIENFELD, AIDAN THOMPSON, Sandia National Laboratories — Alkali nitrate eutectic mixtures are finding application as industrial heat transfer fluids in concentrated solar power generation systems. An important property for such applications is the melting point, or phase coexistence temperature. We have computed melting points for lithium, sodium and potassium nitrate from molecular dynamics simulations using a recently developed method [1-3], which uses thermodynamic integration to compute the free energy difference between the solid and liquid phases. The computed melting point for NaNO3 was within 15K of its experimental value, while for LiNO3 and KNO3, the computed melting points were within 100K of the experimental values [4]. We are currently extending the approach to calculate melting temperatures for binary mixtures of lithium and sodium nitrate.

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