Direct Estimation of the Chemical Potential of Molten NaCl by Molecular Dynamics Simulation

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Molecular dynamics simulation of molten NaCl was carried out at 1200 K with well defined potential parameters. The chemical potential of the melt was satisfactorily estimated with the method proposed by Powles et al., which requires only positional data of the ions at the temperature in question, when the number of ions in the basic cell is large enough.

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