Abstract Submitted
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Computation of free energy of liquids and its application to melting of CO_2 and N[1] AMANUEL TEWELDEBRHAN , Lawrence Livermore National Lab , BRIAN BOATES , STANIMIR BONEV , Dalhousie Univeristy and Lawrence Livermore National Lab — A computationally efficient method is proposed to compute the free energy of liquids with accuracy comparable to *ab initio* thermodynamic integration. The method has been applied to predict melting curves of CO_2 and N over a wide range of pressure using the solid-liquid phase coexistence approach. The calculated melting lines are compared with available experimental data and the crossing of the geotherm and melting line of CO_2 is determined.

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