

New non-empirical approximation for the ionic thermal contribution to the equations of state based on average-atom models

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A new simple approximation for the ionic components of thermodynamic functions is proposed, which reflects the main regularities of their behavior with changes in temperature and density, revealed by analyzing the results of calculations by the pseudoatom molecular dynamics method, and can be employed to calculate the ionic thermal contribution to the equations of state based on average-atom models. It is shown that the use of the new approximation for the ionic contribution instead of the ideal gas or one-component plasma ones significantly improves the accuracy of the Liberman model calculations.