

Ab initio free energy calculation of superionic ice

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Determining the structure and physical properties of ice is an important, ongoing issue in physics, chemistry, geophysics, and planetary science. At extreme high pressure and temperature conditions above 100 GPa and ~2000 K, the existence of the superionic ice has been suggested. However, the structure and physical properties of superionic ice phase are still unknown. Here we introduce our efforts to calculate free energy of superionic ice at high pressure and temperature conditions using ab initio thermodynamic integration method.