Comparison of reliability between first principle simulations and high-pressure experiments

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It is known that the simulation based on the first principles can lead the reliable data at extreme conditions corresponding to the interior of the Earth or planets. However, we do not know the reliability of simulations at high pressures and temperatures where high pressure experiments can not access. Therefore, we have investigated the reliability of ab initio simulations compared with our experimental data. B2-type NaCl was used as a sample in our study. The high-pressure experiments were performed by the diamond anvil cell using the laser heating [1]. The simulations were performed using ab initio molecular dynamics method within the density-functional theory framework [2]. Experimental data acquired at room temperature were likely to be better than those from simulations. In contrast, high-pressure and high-temperature data from experiments did not have any advantages compared with those from simulations. This indicates that a collaborative work between high-pressure experiments and ab initio simulations is better than conventional methods.