First-principles Simulations of LiH: Towards the B2 Phase

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Recent progress in high-pressure experiments has greatly expanded the accessible pressure and temperature conditions, and has proven to be a powerful approach for materials design. However, the characterization of new high-pressure phases is still challenging especially at elevated temperatures. For example, compressing hydrogen to the megabar pressure range is already accessible with laser heated Diamond Anvil Cell (DAC) techniques, yet, it has proven extremely difficult to measure the structural changes upon melting. On the other hand, ab-initio calculation methods, in principle, do not have limitations on the investigation of structural properties under high pressure and temperature conditions. To date, lithium hydride is only the alkali hydride, for which a B2 phase has not yet been found experimentally. The B1-B2 phase boundary at 0 K suggested by previous ab-iniito calculations are around 4 megabar, which is still out of reach for DAC experiments, however, the temperature axis has not yet been explored. We demonstrate, by using an ab-initio two-phase simulation method, that the B1-B2 phase boundary near the melting line is as low as 1.5 megabar, which is within the reach of the laser heated DAC technique.

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