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**First principle study on high pressure phase of LiH: discovery of B2 phase**[1] TADASHI OGITSU, Lawrence Livermore National Laboratory, TADASHI OGITSU TEAM, ERIC SCHWEGLER TEAM, FRANCOIS GYGI TEAM, GIULIA GALLI TEAM — Recent progress in high-pressure experimental method expanded the accessible P-T condition significantly, and it has already been established as a powerful method for material design. However, characterization of the new phase is still challenging especially at high-temperature. For example, melting line of hydrogen under mega bar range is already accessible for laser heated Diamond Anvil Cell (DAC) technique, yet, it is not possible to determine the structural change upon the melt. On the other hand, ab-initio calculation method, in principle, does not have the limitation both in the physical condition and in structural characterization. Lithium hydride is only the alkali hydride, in which B2 phase has not yet been found experimentally. The B1-B2 phase boundary at 0K suggested by previous ab-iniito calculations are around 4 mega bar, which is still out of reach for DAC, however, the temperature axis has not yet been explored yet. We demonstrate, using ab-initio two-phase simulation method, that B1-B2 phase boundary near melting line is as low as 150Gpa, which is accessible with the laser heated DAC method. The detailed discussion will be given at the presentation.

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