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Boson peak, Ioffe-Regel Crossover, and Liquid-Liquid phase transition in Supercooled Water PRADEEP KUMAR, Univ of Arkansas-Fayetteville — We have investigated the onset of Boson peak in a model of liquid water which exhibits a clear first-order phase transition between a low-density liquid phase and a high-density liquid phase of water at low temperature and high pressure. We find that the at low pressures, the onset of Boson peak coincides with the Widom-line of the system. At high pressures, the onset occurs at the transition temperature between the two liquids. Furthermore, we show that at both low and high pressure, the frequency of the Boson peak coincides with the Ioffe-Regel crossover of the transverse phonons, suggesting that the breakdown of Debye behavior is a general feature of Ioffe-Regel limit crossover in supercooled water. The frequency of the Boson peak is weakly pressure dependent and decreases with increasing pressure. Our work bridges gap between the experimental results on the Boson peak nanoconfined water and the behavior that one would expect from a bulk system.

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