Wang *et al.* Reply: In the preceding Comment [1], Formisano and De Panfilis expressed their concerns about the results reported in our Letter [2]. In this Reply, we will address their comments point by point.

The first point is the relation between the boson peak (BP) of the confined water studied in our Letter and the low-frequency excitations observed at ~6 meV (LFE6s) in bulk water with inelastic x-ray scattering (IXS) [3] and in bulk heavy water with inelastic neutron scattering (INS) [4]. The LFE6s are the bumps observed in the coherent dynamic structure factor of the water sample $S_{\mathrm{coh}}(Q,E)$. In the early days, the origin of the LFE6 was tentatively assigned to the O-O-O bending vibrations [5]. The development of the high resolution IXS technique has brought an excellent tool for the investigation of the LFE6. Thorough IXS studies strongly suggest that the LFE6s are collective transverse modes in water [3,6,7]. The BP in the Letter is referred to the bump at ~2–10 meV in the incoherent dynamic structure factor of the confined water $S_{\mathrm{inc}}(Q,E)$. Because of the exceptionally large incoherent cross section of the H atom, the inelastic neutron scattering spectrum of H_2O is dominated by the incoherent signal and thus can be considered as $S_{\mathrm{inc}}(Q,E)$. A similar definition can also be found in a recent computer simulation study [8]. In the literature of amorphous materials, the BP is usually referred to the excess part of the reduced vibrational density of states $g(E)$ over the Debye model [9–11]. Note that, for a classic system, $g(E)$ and $S_{\mathrm{inc}}(Q,E)$ have the following relation [12]:

$$g(E) = \frac{G(E)}{E^2} \propto \lim_{Q\to 0} \frac{S_{\mathrm{inc}}(Q,E)}{Q^2},$$

where $G(E)$ is the vibrational density of states. Recent studies show that the BP is related to the transverse modes [8–10]. However, directly comparing the BP and LFE6, as was done in the preceding Comment, is still improper, since they are related to $S_{\mathrm{inc}}(Q,E)$ and $S_{\mathrm{coh}}(Q,E)$, respectively, and behave differently [9,11]. We emphasize that in our Letter we focus on the BP of the confined water, but not the LFE6 of the confined water.

We disagree with the Comment's argument that the INS approximation is not satisfied at $Q \approx 2.0$ Å^{-1} and that the purely incoherent approximation cannot be uncritically adopted as was done in the Letter. In previous studies it was shown (see, e.g., Ref. [13]) that the INS approximation for materials containing mostly incoherent scattering atoms (like H_2O, where the ratio $\sigma_{\mathrm{inc}}/\sigma_{\mathrm{coh}} = 20.7$) should work well.

The Comment questions the linear interpolation method used in determining T_B. Because of the smooth and monotonic change of the maximum of $\partial_E S_{\mathrm{th}}(Q,E)$ as a function of temperature, the error in this estimation of T_B, evaluated with the method introduced in Ref. [14], is found to be quite small. The Comment also mentions that the peak associated with low frequency has virtually no temperature dependence. This statement is fairly reasonable for the LFE6, the peak observed in $S_{\mathrm{coh}}(Q,E)$ [15], but not for the BP. A recent study on the BP in deeply cooled confined water shows that the temperature dependence of the BP in confined water cannot be ignored [16].

In addition, the Comment points out the difference of the inner pressure and outer pressure induced by the nanoconfinement. We are aware of this difference and we did not directly assign the phase diagram of the confined water to bulk water. In fact, in our recent publications [17,18], we compare the phase diagrams of deeply cooled confined heavy water and deeply cooled bulk heavy water. We find that the liquid-liquid transition lines of these two systems have a pressure difference of ~1 kbar. The order of this difference is consistent with a rough estimation with the Young-Laplace equation.

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[1] F. Formisano and S. De Panfilis, preceding Comment, Phys. Rev. Lett. **115**, 149801 (2015).
[2] Z. Wang, K.-H. Liu, P. Le *et al.*, Phys. Rev. Lett. **112**, 237802 (2014).
[3] F. Sette, G. Ruocco, M. Krisch, C. Masciovecchio, R. Verbeni, and U. Bergmann, Phys. Rev. Lett. **77**, 83 (1996).
[4] C. Petrillo, F. Sacchetti, B. Dorner, and J.-B. Suck, Phys. Rev. E **62**, 3611 (2000).

[5] S. Sastry, F. Sciortino, and H. E. Stanley, J. Chem. Phys. **95**, 7775 (1991).

[6] E. Pontecorvo, M. Krisch, A. Cunsolo, G. Monaco, A. Mermet, R. Verbeni, F. Sette, and G. Ruocco, Phys. Rev. E **71**, 011501 (2005).

[7] A. Cunsolo, G. Ruocco, F. Sette, C. Masciovecchio, A. Mermet, G. Monaco, M. Sampoli, and R. Verbeni, Phys. Rev. Lett. **82**, 775 (1999).

[8] P. Kumar, K. T. Wikfeldt, D. Schlesinger, L. G. M. Pettersson, and H. E. Stanley, Sci. Rep. **3**, 1980 (2013).

[9] H. Shintani and H. Tanaka, Nat. Mater. **7**, 870 (2008).

[10] A. I. Chumakov, G. Monaco, A. Monaco *et al.*, Phys. Rev. Lett. **106**, 225501 (2011).

[11] A. I. Chumakov, I. Sergueev, U. van Bürck, W. Schirmacher, T. Asthalter, R. Rüffer, O. Leupold, and W. Petry, Phys. Rev. Lett. **92**, 245508 (2004).

[12] S.-H. Chen, K. Toukan, C.-K. Loong, D. L. Price, and J. Teixeira, Phys. Rev. Lett. **53**, 1360 (1984).

[13] J. M. Carpenter and C. A. Pelizzari, Phys. Rev. B **12**, 2397 (1975).

[14] https://en.wikipedia.org/wiki/Linear_interpolation.

[15] E. Mamontov, A. De Francesco, F. Formisano, A. Laloni, L. Sani, B. M. Leu, A. H. Said, and A. I. Kolesnikov, J. Phys. Condens. Matter **24**, 064102 (2012).

[16] A. Cupane, M. Fomina, and G. Schirò, J. Chem. Phys. **141**, 18C510 (2014).

[17] Z. Wang, K.-H. Liu, L. Harriger, J. B. Leão, and S.-H. Chen, J. Chem. Phys. **141**, 014501 (2014).

[18] Z. Wang, K. Ito, J. B. Leão, L. Harriger, Y. Liu, and S.-H. Chen, J. Phys. Chem. Lett. **6**, 2009 (2015).