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Title
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In Ref. 1 we present and analyze experimental high resolution x-ray emission spectra (XES) of liquid water which exhibit a splitting of the $1b_1$ line into two components. We also suggest a qualitative model to explain the experimental spectra which, even though tentative (as clearly stated in the summary of Ref. 1), is able to explain ALL available experimental data. In the meantime we have collected new data[2], which further support and strengthen our model (see below).

Pettersson et al. claim that a spectrum with two similarly sharp $1b_1$ features both from a dissociated product (d_2) and from the intact molecule (d_1) would be "unphysical and unsubstantiated" since "the path connecting initial and final structure" is not taken into account. In contrast, it was reported[3] that the dissociation of a molecule (HCl) during the core-hole lifetime can indeed lead to two distinct peaks. In Ref. 3, these peaks have very different widths since the dissociated atomic-like product (Cl^-) exhibits no vibrational broadening whereas the intact molecule (HCl) does. In our case, both the intact molecule (H_2O) and its dissociated product are expected to exhibit a vibrational broadening which is consistent with our observation of two lines with similar widths. Similar to our model, dissociation of water during the core hole lifetime was previously observed using resonant Auger spectroscopy[4]. Note that intermediate states may still be part of the spectra, but their spectral weight can be rather small, as explained in Ref. 3.

In their comment, Pettersson et al. use Density Functional Theory (DFT) to simulate the core hole-induced dynamics in XES spectra of water. We note that all DFT calculations to date, including those by Pettersson et al., do not predict a splitting of the $1b_1$ emission line.[5] Note that there is even still a controversy on simulating the (dynamics-free and thus much simpler) X-ray absorption spectra (XAS) of liquid water.[6,7] In their comment, Pettersson et al. list an accepted manuscript[8] in which DFT calculations, inspired by the experimental results, indeed now reproduce a $1b_1$ splitting, but only under the assumption of very specific hydrogen bonding configurations and a questionable explanation of the isotope effect.

Furthermore, Pettersson et al. correctly argue that the d_2 component is expected to increase in its spectral weight when going from non-resonant to resonant excitation into the pre-edge (534.6 eV). Contrary to what Pettersson et al. claim, this is exactly what our experimental data in Ref. 1 show. Moreover, our newer data set in Fig. 1 (adapted from Ref. 2), shows the XES intensity in a color-coded 2-D diagram as a function of excitation and emission energies. It is evident that the high-energy $1b_1$ component d_1 (emission energy 527.5 eV) exhibits a Raman-like shift, but vanishes when exciting into the pre-edge, while the d_2 component still has a strong intensity (and does not exhibit a Raman-like shift until the onset of the pre-edge excitation is reached).

Pettersson et al. also claim that Raman shifts make it impossible to compare resonantly excited NaOH spectra with non-resonantly excited water spectra. This argument is not valid in the present case, since all spectra being compared were taken at excitation energies above the Raman regime. As clearly visible in Fig. 1, no Raman-like shifts are observed for liquid water in the relevant photon energy range. Furthermore, our data for the resonant pre-pre-edge region of NaOH (to be published) shows no significant Raman shift, indicating that a comparison of resonant and non-resonant spectra is entirely appropriate in our case.

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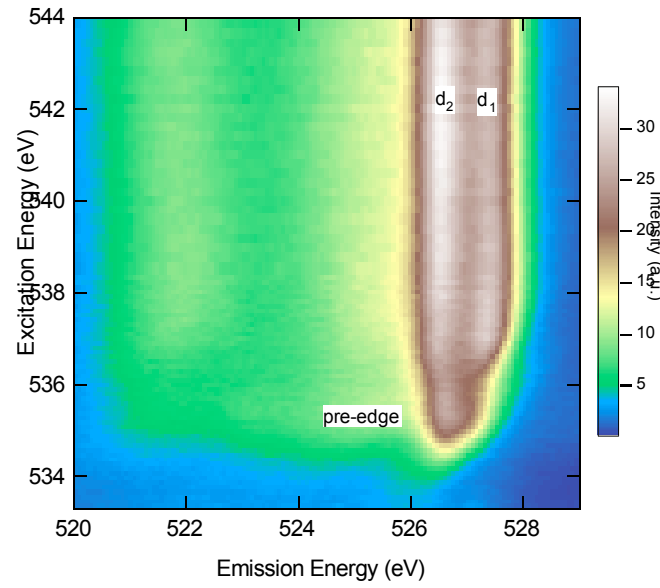[8]T. Tokushima et al., http://dx.doi.org/10.1016/j.cplett.2008.04.077

Fig. 1: Resonant x-ray emission intensity of water as a function of excitation and emission energy. d_1 and d_2 denote the two $1b_1$ components. Figure modified from Ref. 2.