

Dissociation of water molecules after $O1s \rightarrow 4a_1$ excitation

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Water is one of the most studied of all the small molecules. After all, it is essential for all forms of life on Earth. The presence of water and carbondioxide in our atmosphere provides us a climate favorable for living. Water is also one of the most abundant molecules on Earth and has therefore been used in a wide variety of applications not least because of the extraordinary physical and chemical properties of water molecules. The small size of the molecule (only ten electrons) has increased its popularity as a showcase system for theoretical studies.

The lowest unoccupied molecular orbital (LUMO) in water is an antibonding $4a_1$ orbital and excitation of the $O1s$ core-electron to this orbital leads to dissociation, which has been shown to take place on a femtosecond timescale [1]. In order to understand the process in more detail, we have performed photoelectron-photoion-coincidence measurements using synchrotron radiation with a setup described in [2]. Experimental results allowed us to study how the dissociation depends on the final electronic states involved in the resonant Auger decay followed by the core-excitation.

Potential energy curves of the excited state as well as the electronic final states of the resulting ion from quantum chemical calculations performed with MOLCAS package [3] have been used in the interpretation of the experimental results. Combining the information obtained from coincidence experiments and quantum chemical calculations we can reveal details of the different dissociation processes related to different electronic final states of water ion.

References:

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