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Atmospheric iodine oxide surface propensity determined by combined theoretical calculations and liquid jet XPS

Content

Iodine chemistry is implicated in atmospheric chemistry and can form several oxides such as HOI, I2, IO, OIO, and finally I2O5 or HIO3, which may nucleate as nanoparticles relevant for cloud formation in remote environments (Saiz-Lopez et al., 2012). These oxides can be formed through reaction with oxidants or other halogen compounds in the gas phase or the particle phase. Most of the iodide oxidation processes have been suggested to be enhanced at interfaces, similar to those involving other halogen species, either due to the surface propensity of intermediates (Artiglia et al., 2017) or the iodine species itself (Moreno and Beaza-Romero, 2019). However, no data are available about the surface concentration of iodine species other than iodide. After two decades of research into the surface propensity of iodide and bromide, the picture emerges that their surface propensity is not as extreme as initially thought (Jungwirth and Tobias, 2002; Ghosal et al., 2005; Olivieri et al., 2018).

Liquid jet X-ray photoelectron spectroscopy (XPS) experiments have been carried out at the SIM beamline at the Swiss Light Source. Acquisition of kinetic energy dependent (thus at different probing depth) I3d, I4d core level and valence level spectra has been done for iodide, iodate and iodic acid. This allows to retrieve the surface propensity of these iodine species at the aqueous solution – air interface. HIO3, HOI and iodide surface propensity has also been investigated by Ab Initio Molecular Dynamics computation using CP2K software. Finally, binding energies in aqueous phase are compared to theoretical computations using the so-called Frozen Embedding Method where DFT SAOP is coupled with CVS-EOM-IP-CCSD/d-aug-dy-all.ac2vz via a molecular mean-field X2C including the Gaunt interaction (Halbert et al., 2020).

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