

Abstract template:

**Title**

Sum Frequency Generation surface spectra of ice, water and acid solution investigated by an exciton model

**Reference**

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**Authors**

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**Abstract**

A new computational scheme is presented for calculation of sum frequency generation –SFG– spectra, based on the exciton model for OH bonds. The scheme is applied to unified analysis of the SFG spectra in the OH-stretch region of the surfaces of ice, liquid water, and acid solution. A significant role of intermolecularly coupled collective modes is pointed out. SFG intensity amplification observed for acid solutions in the H-bonded OH-stretch region is reproduced qualitatively and accounted for by enhanced orientational preference “into the surface” of the H<sub>2</sub>O bisectors within the hydronium solvation shell.