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Sum frequency generation spectra of ice surfaces from first principles simulations[1] QUAN WAN, University of California Davis and The University of Chicago, FRANCOIS GYGI, University of California Davis, GIULIA GALLI, The University of Chicago — The morphology and structure of ice surfaces play an important role in a variety of chemical and physical processes. Yet a detailed knowledge of the structural properties of ice surfaces at the molecular level is still lacking. Sum frequency generation (SFG) spectroscopy is a promising technique to address this problem, due to its high interface sensitivity. Here we present first principles simulations of SFG spectra of ice surfaces obtained by *ab initio* molecular dynamics, combined with density functional perturbation theory (DFPT), as implemented in the Qbox Code. We computed SFG signals from classical time correlation functions of the system's dipole moment and polarizability tensor, evaluated by using maximally localized Wannier functions and DFPT. By projecting the total SFG intensities onto each molecules, we analyzed the stretching band region of the SFG spectra and identified intra- and inter-bilayer modes. This analysis was then used to shed light on whether the ice surface is proton ordered or disordered. In addition to ice, we will also discuss simulations of SFG signals obtained for solid-water interfaces using the same *ab initio* method.

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