VSFG spectrum from classical molecular dynamics simulations: Alumina (0001) and Fluorite (111) Surfaces

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Introduction

Vibrational Sum Frequency Generation (VSFG) is well established experimental method that can explore processes on various water/solid interfaces. Hand in hand with development of this experimental technique theoretical approaches to get SFG spectrum from classical and ab-initio molecular dynamic simulations have arisen. Recently, new approach that uses velocity-velocity correlation functions (VVCF) to calculate VSFG spectra [1] was demostrated to properly describe VSFG spectrum of a fluorite surface using *ab-initio* molecular dynamics (AIMD). The advantage of this method is that it only requires the atomic positions and velocities without the cost of calculation of molecular dipoles and polarizabilities in each step.

Results

We have adopted the method based on VVCF and explored posibilities of the phase-resolved VSFG spectra prediction from *classical* MD simulations (CMD). Performance of various flexible water models based on well-established SPC and TIP3P models was compared to predict VSFG spectra of the alumina (0001) and fluorite (111) surfaces corresponding to a range of pH values. Results show good agreement between CMD computed spectra and AIMD computed or experimental ones. Of course, with much less computational effort in the case of CMD simulations compared to AIMD ones.

[1] Khatib *et al.* (2016) Sci. Rep. 6, 24287