Optimization of quartz-enhanced photoacoustic spectroscopy sensor for isotopologue analysis using ab initio calculations

Blythe Ashcraft[1], S. McWhorter[1], A.A. Kosterev[2], R. Lascola[1], F.K. Tittel[2]; [1]Savannah River National Laboratory; [2]Rice University

The Savannah River Site (SRS) has a long history of hydrogen isotopic processing and analysis. Real-time monitoring of trace impurity formation is vital to optimization of the hydrogen processing conditions. Isotopologues of ammonia, methane, and water are known or expected impurities in the processing of hydrogen isotopes. Researchers at the Savannah River National Laboratory (SRNL) and Rice University have been developing quartz enhanced photoacoustic spectroscopy (QEPAS) sensors for trace gas sensing in a hydrogen process stream. QEPAS is a variation of conventional PAS which utilizes a piezo-electric tuning fork coupled with a quartz resonator. Given the lack of readily available literature concerning the vibrational spectra of the impurity isotopologues, computational modeling was utilized to determine an optimal laser tuning range for the experiments. This presentation will outline the principles of QEPAS and recent experimental results including detection of ammonia and methane in a hydrogen gas stream along with results from computational calculations.