

# Quantum Ocean: Charactering Deep Ocean Water using Density Function Theory and Raman Spectroscopy

S F DIMARCO<sup>1</sup>, N ALTANGEREL<sup>2</sup>, A HAZRATHOSSEINI<sup>2</sup>, A H KNAP<sup>1</sup>, Y LIU<sup>1</sup>, S HSU<sup>3</sup>, P R HEMMER<sup>2</sup>, A M ZHELTIKOV<sup>2</sup>, A V SOKOLOV<sup>2</sup>, AND M O SCULLY<sup>2</sup>

<sup>1</sup>*Geochemical and Environmental Research Group, Texas A&M University, College Station, TX, USA*

<sup>2</sup>*Institute for Quantum Science and Engineering, Texas A&M University, College Station, TX, USA*

<sup>3</sup>*Oceanography, Texas A&M University, College Station, TX, USA*

Contact Email: [sdimarco@tamu.edu](mailto:sdimarco@tamu.edu)

Advancements in quantum technology, sensing, and computation have the potential to provide observational solutions of the subsurface ocean with unprecedented accuracy and precision, which will advance understanding, innovation, and lead to improved prediction of the natural world. Computationally-predicted vibrational signatures calculated using density functional theory (DFT) of pure water and salt water are used to interpret experimental Raman spectra of in situ water samples collected in the Gulf of Mexico. Spectra from independent Raman spectra methodologies are compared: surface enhanced Raman Spectroscopy (SERS) and a handheld Raman spectrometer. Results show key differences in the Raman spectra (range: 500-1500  $\text{cm}^{-1}$ ) of deepwater (*i.e.*, high salinity,  $\sim 35$  ppt) and shallow (*i.e.*, low salinity,  $\sim 1-2$  ppt) locations. Additional characterization of oceanographic nutrient constituents (*e.g.*, phosphate) and presence of multiple protein species and nucleic acids in the ocean samples re-enforce this technique's potential to unlock new mechanistic basis for oceanographic processes and their interaction. Validation of the SERS spectra with that measured using the portable device provides a pathway for assessing the suitability of such devices on autonomous ocean observing platforms, which require low power, light-weight, and weather-ready solutions.