Computational approach to glucose detection with SERS

Diabetes mellitus is a group of metabolic disorders resulting in an abnormally elevated level of glucose in the blood. Continues monitoring of blood sugar's level is critically important to prevent diabetes complications. Although different types of glucose sensing methods have been investigated, the existing methods of measurements have substantial problems. In demand for better sensing approaches, optical technologies have been explored of which Surfaced Enhanced Raman Scattering (SERS) yielding superior functionality. In this work, we have established glucose sensing method by tracking the glucose-induced shift in the SERS emission of 4-Mercaptophenyl Boronic Acid (MPBA) on the flat surface of gold using Density Functional Theory (DFT) simulation. The existing literatures suggest that MPBA exists in two distinct form: MPBA and charged (OH-)-associated MPBA, with the relative contributions strongly depends on the pH value. Our SERS calculations for MPBA resolve both configurations of MPBA and confirm the co-existence of both forms in experimental data. The SERS of MPBA has two major peaks around 1100 cm^{-1} and 1600 cm^{-1}, which the latter is highly pH dependent, unlike the former. By bonding glucose on MPBA, the two major peaks coexist, nevertheless the peak around 1100 cm^{-1} moves to slightly higher wavenumber, as confirms by both experiment and theoretical calculations. The vibrational modes study of the designated peak shows that bonding glucose to the linker, suppresses the "breathing" mode of MPBA and energizes the "constrained-bending" mode at higher wavenumber, causing the dominant peak to shift.