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Analysis of Serotonin Molecules on Silver Nanocolloids – a Raman Computational and Experimental Study EMMA SUNDIN, University of Texas at El Paso, Department of Biomedical Engineering, JOHN CIUBUC, Department of Biomedical Engineering, KEVIN BENNET, Mayo Clinic, Division of Engineering, Department of Neurologic Surgery, Rochester MN 55905 USA, FELICIA MANCIU, University of Texas at El Paso, Department of Physics, Border Biomedical Research Center, El Paso TX 79968 USA — The neurotransmitter serotonin is found throughout the human body and serves numerous functions, but is found physiologically in very low concentrations. To better understand issues surrounding detection and monitoring of serotonin at such levels, this study combines quantum chemical density functional modeling and surface-enhanced Raman spectroscopy. The ultrasensitive experimental analyte detection at 10^{-11} molar concentrations is in relatively good agreement with the modeled results. The simulation results indicate the presence of all serotonin molecular forms, including neutral, ionic, and redox-reaction oxidized forms. Furthermore, ionic and oxidized forms were found to exhibit molecular deformations such as bending of amine chains. Serotonin is thus revealed, by this combined approach, to absorb with greater probability onto the silver surface at its hydroxyl/oxygen sites than through NH/nitrogen sites, and to absorb more readily in its neutral (reduced) form than in its ionic forms. By investigating the vibrational signatures of this important neurotransmitter, this study furnishes some necessary background for future advancements in opto-voltammetric biosensors.

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