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Ultrasensitive Detection of Dopamine by Combined Theoretical and Experimental Raman Studies FELICIA MANCIU, University of Texas at El Paso, Department of Physics, Border Biomedical Research Center, El Paso TX 79968 USA — Detection of trace amounts of neurotransmitters has become significant in diagnostic applications. Theoretical and experimental analysis of dopamine (DA) at sub-nanomolar concentrations relevant to physiological levels is presented in this work. Surface-enhanced Raman spectroscopy (SERS) utilizing silver nanoparticles was used for experimental studies and quantum chemical density functional methods for calculations. The relatively good agreement between the simulated and experimental results suggests the possibility that different forms of the DA molecule, such as uncharged $DA^{\pm}$, anionic DA^{-}, and dopaminequinone are simultaneously present. All of these molecular configurations, in a SERS environment, lose the dominant DA Raman lines at 750 $cm^{-1}$and 790 cm^{-1}. The occurrence of these features would imply the potential presence of multilayer neutral DA^{0}, or that of cationic DA^{+}. From a redox reaction perspective, the dopaminequinone form is more likely detected during the oxidation process, while the $DA^{\pm}$ form probably occurs during reduction. The ultrasensitivity demonstrated in the experimental data, in combination with the theoretical analysis presented, provides valuable information for advancing the detection and monitoring of DA.

Felicia Manciu
The University of Texas at El Paso

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