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Quantum confined Stark effect in organic fluorophores. XIHONG PENG, Rensselaer Polytechnic Institute (RPI), JOHN ANDERSON, US Army Corps of Engineers, GARY TEPPER, SUPRIYO BANDYOPADHYAY, Virginia Commonwealth Univ, SAROJ NAYAK, RPI — Fluorescent molecules have widely been used to detect and visualize structure and processes in biological samples due to its extraordinary sensitivity. However, the emission spectra of flurophores are usually broad and the accurate identification is difficult. Recently, experiments show that energy shifts by Stark effect can be used to aid the identification of organic molecules [1]. Stark effect originates from the shifting/splitting of energy levels when a molecule is under an external electric field, which shows a shift/splitting of a peak in absorption/emission spectra. The size of the shift depends on the magnitude of the external field and the molecular structure. In this talk we will show our theoretical study of the peak shifts on emission spectra for a series of organic fluorophores such as tyrosine, tryptophan, rhodamine123 and coumarin314 using density functional theory. We find that a particular peak shift is determined by the local dipole moments of molecular orbitals rather than the global dipole moment of the molecule. These molecular-specific shifts in emission spectra may enable to improve molecular identification in biosensors. Our results will be compared with experimental data. [1]Unpublished, S. Sarkar, B. Kanchibotla, S. Bandyopadhyay, G. Tepper, J. Edwards, J. Anderson, and R. Kessick.

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