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Use of Ultrafast Molecular Dynamics and Optimal Control for Identifying Biomolecules

JEAN-PIERRE WOLF, University of Geneva

With F.COURVOISIER,L.GUYON,V.BOUTOU, and M.ROTH,J. ROSLUND, H. RABITZ, Princeton University. The identification and discrimination of molecules that exhibit almost identical structures and spectra using fluorescence spectroscopy is considered quite difficult. In order to evaluate the capability of optimal control for discriminating between the optical emissions of nearly identical molecules, we developed a new approach called "optimal dynamic discrimination (ODD). A proof of principle ODD experiment has been performed using Riboflavin (RBF) and Flavin Mononucleotide (FMN) as model system. We used a complex multipulse control field made of a pair of pulses (UV and IR). The UV part (400 nm) is optimally shaped using a control learning loop while the IR component (800 nm) is FT-limited (100 fs) and set at a definite time delay with respect to the UV pulse. Clear discrimination was observed for optimally shaped pulses, although the linear spectra from both molecules are virtually identical. A further experiment showed that, by using the optimal pulse shapes that maximize the fluorescence depletion in FMN and RBF in a differential manner, the concentration of both molecules could be retrieved while they were mixed in the same solution. The ODD demonstration sets out a promising path for future applications, as for example fluorescence microscopy where endogenous fluorescence spectra of many biomolecules overlap.