Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

'Exotic' Electron Spectroscopy of Molecules in Electric Fields[1]
RAJEEV PATHAK, NALINI GURAV, Department of Physics, S. P. Pune University, Pune, MH 411007, India, SHRIDHAR GEJJI, Department of Chemistry, S. P. Pune University, Pune, MH 411007, India — Single molecules, whether polar or non-polar (in their free state), when subjected to an externally applied uniform electric field, are observed to exhibit remarkably different UV spectra from those of their zero-field counterparts. Significant spectral line-shifts, line-splitting, line-merging as well as disappearance, and emergence of 'exotic' spectral lines are observed as a function of the applied electric field strength. In particular, we simulate the molecular electronic-transition spectra of methanol, hydrogen-peroxide, water and carbon-dioxide in an electric field, employing time dependent density functional theory (TD-DFT) under the versatile M06-2X dispersion-corrected DFT prescription. It is further demonstrated that the Natural Localized Molecular Orbitals (NLMOs), playing a dual donor-acceptor role, can best describe the electron density redistribution and the interplay of various bands in the UV spectrum which is traced back to mutations and crossings of the frontier molecular orbitals.

[1]We would like to thank the Center for Advanced Computing, Pune University Campus, for computer time.

Rajeev Pathak
Department of Physics, S. P. Pune University, Pune, MH 411007, India

Date submitted: 22 Sep 2016 Electronic form version 1.4