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***Ab initio* studies on molecules and clusters in external electrostatic fields** RAJEEV PATHAK, Department of Physics, University of Pune, Pune 411007, Maharashtra, India — Influence of a uniform static external electric field on some aliphatic and aromatic molecular species is studied within the density functional theory (DFT) employing the 6-311++G(2d,2p) basis-set with B3LYP exchange-correlation prescription. The electric field perturbs the molecular geometry; alters the dipole moments and engenders a molecular vibrational Stark effect. For polar molecules, significant frequency shifts are observed for field orientations both parallel and antiparallel to their permanent dipole moments; where HOMO-LUMO gaps alter significantly. Time dependent DFT analysis reveals that an increase in the applied field strength increases the excitation energies amongst frontier MOs with a concomitant decrease in oscillator strengths. Structural evolution of water clusters, $(H_2O)_n$, n=6-8 is studied within DFT: the intermolecular hydrogen bonds stretch, and eventually break at some threshold values, triggering a conformational transformation, with configurations appearing as local minima on the cluster's potential energy landscape, with abrupt increase in the electric dipole moments and 'opening up' of three dimensional morphologies of water.

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