Title:	Linearizing Water Molecule Using A Linearly Polarized High Intensity High Frequency Laser
Authors:	Tiwari, Vishal (/jspui/browse?type=author&value=Tiwari%2C+Vishal)
Issue Date:	10-Oct-2019
Abstract:	The work presented in this thesis addresses the possibility of trapping water molecule in a linear geometry in the presence of high-frequency, high-intensity electromagnetic radiation. Chapter 1 of the thesis starts with a basic review of the literature, giving a description of Multiphoton ionization, Above-threshold ionization, Tunnel ionization and Higher harmonic generation in strong field interactions in molecules, together with a motivation of the problem . In Chapter 2, the reason for the question is analyzed. Using solutions of time independent Schrödinger equation in the oscillating frame of reference, it is shown that a linear geometry of water molecule is favoured over the bent geometry. The reason for this stabilization is then analyzed in terms of Kramers-Henneberger(KH) potential and orbital interactions as a function of laser parameters and geometry. Using Hartree Fock and Configuration Interaction Singles calculations at a converged all electron basis set, it is found that the stabilization of the linear goemetry is 23.89 eV . In Chapter 3, time dependent calculations using a modified (t, t) method has been done in presence of electric field with aforementioned laser parameters in a sin 2 envelope with the Continuous Wave region in between the rise and fall of pulse. Electronic wavepacket dynamics of water molecule is done with a realistic laser pulse of peak intensity 2.2464 × 10 14 W/cm 2 and frequency of 431 nm. The time average of the energy over the Continuous Wave region of the pulse is found to be lesser for the linear geometry indicating its stabilzation. In contrast to 800 nm and a similar intensity giving ionization, in the off resonant 431 nm pulse with a rise time of 0.96 f s and pulse duration of 2.88 f s the stabilization is achieved and maintained.
URI:	http://hdl.handle.net/123456789/1262 (http://hdl.handle.net/123456789/1262)
Appears in Collections:	MS-14 (/jspui/handle/123456789/1078)

Files in This Item:

File	Description	Size	Format	
MS14017.pdf (/jspui/bitstream/123456789/1262/3/MS14017.pdf)	Full Text.pdf	2.96 MB	Adobe PDF	View/Open (/jspui/bitstream/123456789/1262/3/

Show full item record (/jspui/handle/123456789/1262?mode=full)

(/jspui/handle/123456789/1262/statistics)