

**Ultrafast Nonadiabatic Fragmentation Dynamics of Doubly Charged Uracil in a Gas Phase**  
**Lopez-Tarifa P. ; du Penhoat M. -A. Herve ; Vuilleumier R. ; et al., PHYSICAL**  
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BECKE AD DENSITY-FUNCTIONAL EXCHANGE-ENERGY APPROXIMATION WITH CORRECT ASYMPTOTIC BEHAVIOR PHYSICAL REVIEW A 38(6) 3098 DOI: 10.1103/PhysRevA.38.3098 1988

Cafarelli P et al. Ionization and Fragmentation of 5-Chlorouracil induced by 100 keV protons collisions Tokesi K; Sulik B 5th International Conference on Radiation Damage in Biomolecular Systems Debrecen, HUNGARY JUN 13-15 2008 RADIATION DAMAGE IN BIOMOLECULAR SYSTEMS AIP Conference Proceedings 71 DOI: 10.1063/1.3058990 2008

Couper B; et al. Inelastic interactions of protons and electrons with biologically relevant molecules EUROPEAN PHYSICAL JOURNAL D 20(3) 459 DOI: 10.1140/epjd/e2002-00166-3 2002

de Vries J; et al. q+-induced excitation and fragmentation of uracil: effects of the projectile electronic structure JOURNAL OF PHYSICS B-ATOMIC MOLECULAR AND OPTICAL PHYSICS 35(21) 4373 PII S0953-4075(02)38596-1 DOI: 10.1088/0953-4075/35/21/304 2002

de Vries J.; et al. Ionization and fragmentation modes of nucleobases after collisions with multiply charged ions PHYSICA SCRIPTA T110 336 DOI: 10.1238/Physica.Topical.110a00336 2004

de Vries J; et al. Charge driven fragmentation of nucleobases PHYSICAL REVIEW LETTERS 91(5) 053401 DOI: 10.1103/PhysRevLett.91.053401 2003

Deng ZW; et al. Beyond the Bragg peak: Hyperthermal heavy ion damage to DNA components PHYSICAL REVIEW LETTERS 95(15) 153201 DOI: 10.1103/PhysRevLett.95.153201 2005

Denifl S; et al. Threshold electron impact ionization studies of uracil INTERNATIONAL JOURNAL OF MASS SPECTROMETRY 238(1) 47 DOI: 10.1016/j.ijms.2004.07.010 2004

Fokas Ernmanouil; et al. Ion beam radiobiology and cancer: Time to update ourselves BIOCHIMICA ET BIOPHYSICA ACTA-REVIEWS ON CANCER 1796(2) 216 DOI: 10.1016/j.bbcan.2009.07.005 2009

Jochims HW; et al. Photoion mass spectrometry of adenine, thymine and uracil in the 6-22 eV photon energy range CHEMICAL PHYSICS 314(1-3) 263 DOI: 10.1016/j.chemphys.2005.03.008 2005

LEE CT; et al. DEVELOPMENT OF THE COLLE-SALVETTI CORRELATION-ENERGY FORMULA INTO A FUNCTIONAL OF THE ELECTRON-DENSITY PHYSICAL REVIEW B 37(2) 785 DOI: 10.1103/PhysRevB.37.785 1988

Liu B.; et al. Collision-induced dissociation of hydrated adenosine monophosphate nucleotide ions: Protection of the ion in water nanoclusters PHYSICAL REVIEW LETTERS 97(13) 133401 DOI: 10.1103/PhysRevLett.97.133401 2006

Moretto-Capelle Patrick; et al. Electron spectroscopy in proton collisions with dry gas-phase uracil base PHYSICAL REVIEW A 74(6) 062705 DOI: 10.1103/PhysRevA.74.062705 2006

Nuevo Michel; et al. Formation of Uracil from the Ultraviolet Photo-Irradiation of Pyrimidine in Pure H<sub>2</sub>O Ices ASTROBIOLOGY 9(7) 683 DOI: 10.1089/ast.2008.0324 2009

RUNGE E; et al. DENSITY-FUNCTIONAL THEORY FOR TIME-DEPENDENT SYSTEMS PHYSICAL REVIEW LETTERS 52(12) 997 DOI: 10.1103/PhysRevLett.52.997 1984

Schlatholter T; et al. Charge driven fragmentation of biologically relevant molecules INTERNATIONAL JOURNAL OF MASS SPECTROMETRY 233(1-3) 173 DOI: 10.1016/j.ijms.2003.12.029 2004

TABET J PHYS REV A 2010

Tang W.; et al. A grid-based Bader analysis algorithm without lattice bias JOURNAL OF PHYSICS-CONDENSED MATTER 21(8) 084204 DOI: 10.1088/0953-8984/21/8/084204 2009

Tavernelli I; et al. Molecular dynamics in electronically excited states using time-dependent density functional theory MOLECULAR PHYSICS 103(6-8) 963 DOI: 10.1080/ 2005

Tavernelli Ivano; et al. Time-dependent density functional theory molecular dynamics simulations of liquid water radiolysis CHEMPHYSCHM 9(14) 2099 DOI: 10.1002/cphc.200800177 2008

TROULLIER N; et al. EFFICIENT PSEUDOPOTENTIALS FOR PLANE-WAVE CALCULATIONS  
PHYSICAL REVIEW B 43(3) 1993 DOI: 10.1103/PhysRevB.43.1993 1991