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Mapping the dissociative ionization dynamics of molecular nitrogen with attosecond resolution

M. Klinker^{1,1}, A. Trabattoni², J. González-Vázquez¹, C. Liu³, G. Sansone², R. Linguerrri⁴, M. Hochlaf⁴, J. Klei⁵, M. J. J. Vrakking⁵, F. Martin^{1,6,7}, M. Nisoli^{2,8}, F. Calegari⁸

¹ Departamento de Química, Módulo 13, Universidad Autónoma de Madrid, Cantoblanco 28049, Madrid, Spain. ² Dipartimento di Fisica di Milano, Piazza Leonardo da Vinci 32, I-20133 Milano, Italy. ³ State Key Laboratory of High Field Physics, Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, Shanghai 201800, China. ⁴ Université Paris-Est, Laboratoire Modélisation et Simulation Multi Echelle, MSME UMR 8208 CNRS, 5bd Descartes, 77454 Marne-La-Vallée, France. ⁵ Max-Born-Institut, Max Born Straße 2A, D-12489 Berlin, Germany. ⁶ Instituto Madrileño de Estudios Avanzados en Nanociencia (IMDEA-Nano), Ciudad Universitaria de Cantoblanco, 28049 Madrid, Spain. ⁷ Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, 28049 Madrid, Spain. ⁸ Institute for Photonics and Nanotechnologies, IFN-CNR, Piazza Leonardo da Vinci 32, I-20133 Milano, Italy.

Synopsis We wish to understand the processes underlying the ionization dynamics of N₂ as experimentally induced and studied by recording the kinetic energy release (KER) in a XUV-pump/IR-probe setup. To this end a theoretical model was developed describing the ionization process using Dyson Orbitals and, subsequently, the dissociation process using a large set of diabatic potential energy surfaces (PES) on which to propagate. From said set of PES, a small subset is extracted allowing for the identification of one and two photon processes chiefly responsible for the experimentally observed features.

N₂ is the most abundant element in the earth's atmosphere and as such is of integral importance to processes induced by solar radiation, in particular the dissociation of N₂ induced by solar XUV light in the upper atmosphere. Recent advances in atto second technology have made it possible to gain new insights into ultra fast electron dynamics following sudden removal of an electron [1, 2], providing the perfect tools to study the photo induced dissociation of N₂.

We present the experimental and theoretical investigation of the ionization and dissociation dynamics of N₂. Isolated attosecond pulses (energy range: 16-50 eV, duration: 300 as) were used to ionize N₂ molecules, through a single photon transition. After a variable delay, 4-fs NIR/VIS CEP controlled pulses (peak intensity: $8 \cdot 10^{12}$ W/cm²) were used to probe the subsequent dissociation dynamics. The angularly resolved momentum distribution of the produced N⁺ fragments was measured as a function of the pump-probe delay using a velocity map imaging (VMI) spectrometer. We observed a depletion of a quasi-bound state of N₂⁺, 8 fs after zero time delay, together with sub-cycle modulation of the N⁺ yield.

To understand the origin of the dynamics a model was developed: The ionization process was simulated assuming an instantaneous transition of the nuclear ground state wave function of N₂ to a set of diabatic PESs of the N₂⁺ ion, obtained us-

ing *ab initio* multiconfigurational methodology. The relative initial populations of said set of ionic PESs were approximated using Dyson orbitals in first order perturbation theory [3, 4] and modelling the leaving electron by a Coulomb wave. The dissociating ion subjected to the IR pulse was modelled by solving the TDSE using Split Operator [5] and Fast Fourier [6] techniques.

Careful investigation of the data produced by aforementioned techniques yielded the F²Σ_g, 3²Σ_g, C²Σ_u and 5²Σ_u states of N₂⁺ as being capable of describing most features observed experimentally; most importantly a two photon transition from F²Σ_g to 3²Σ_g via 5²Σ_u was found to be responsible for the sub-femtosecond dynamics, as it causes the wave packets initially in F²Σ_g and 3²Σ_g to interfere.

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¹E-mail: m.klinker@uam.es

