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In this study it has been carried out theoretical simulations of ab-initio molecular dynamics of the C-H photo-dissociation of methane induced by femtosecond laser pulses. Our discussion about the reaction mechanism leading to the formation of the H and CH_3 fragments is based on the rectification of the Lorentz force.

Fragmentation dynamics of methane induced by femtosecond ...

fragmentation can occur. In the present work, we investigate theoretically, through ab-initio molecular dynamics simulations, the chemical reaction of dissociation of methane induced by intense femtosecond IR pulses. An alternative mechanism based on the

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In this study it has been carried out theoretical simulations of ab-initio molecular dynamics of the C-H photo-dissociation of methane induced by femtosecond laser pulses. Our discussion about the reaction mechanism leading to the formation of the H and CH_3 fragments is based on the rectification of the Lorentz force. Such an electric force rectification occurs via a ...

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Fragmentation dynamics of methane induced by femtosecond laser pulses. Applied Physics B 2016, 122 DOI: 10.1007/s00340-015-6303-x. Su-Yeon Choi, Bong-Ki Ryu. Effects of crystallization on the structural, electrical, and catalytic properties of 75V 2 O 5 -15B 2 O 3 -10P 2 O 5 glass. Journal of Non-Crystalline Solids 2016, 431, 112-117.

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The results demonstrated that the first-return recollision between the rescattered electron and the parent ion played a significant role in the fragmentation dynamics of the parent ion. Depending...

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Instantaneous (laser-field-dependent) potential energy curves leading to neutral fragmentations of methane were calculated at several laser intensities from 1.4 × 10¹³ to 1.2 × 10¹⁴ W/cm² (from 1.0 × 10¹⁰ to 3.0 × 10¹⁰ V/m) using ab initio molecular orbital (MO) methods to validate the observation of neutral fragmentations induced by intense femtosecond IR pulses (Kong et al. J. Chem. Phys. 2006, 125, 133320).

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The fragmentation of CH₄²⁺ dications following 55 eV, 75 eV, and 100 eV electron impact double ionization of methane was studied using a cold target recoil-ion momentum spectroscopy. From the measured momentum of each recoil ion, the momentum of the neutral particles has been deduced and the kinetic energy release distribution for the different fragmentation channels has been obtained.

Fragmentation mechanisms for methane induced by 55 eV, 75 ...

Abstract. The fragmentation pattern of CH₄²⁺ was experimentally studied at an intensity of approximately 10¹⁴ W/cm² with laser durations varying from 80 to 10 fs. When the laser duration was 8 fs, only the primarily fragmental CH₃⁺ ion was observed in addition to the parent CH₄⁺ ion. When the laser duration was 30 fs, small fragmental CH₂⁺ and H⁺ ions appeared. When the laser duration was ...

Fragmentation dynamics of methane by few-cycle femtosecond ...

the fragmentation of the methane molecule, which has attracted a lot of attention due to the tetrahedral structure of its ground state. In particular, the fragmentation has been induced by electrons [1]–[4], protons [5], atoms [6]–[8], synchrotron radiation [9]–[13] and lasers [14, 15].

The role of the methyl ion in the fragmentation of

A momentum imaging spectrometer has been built for studying the electron impact molecular fragmentation dynamics. The setup consists of a pulsed electron gun and a time of flight system as well as a two-dimensional time and position sensitive multi-hit detector. The charged fragments with kinetic ...

Momentum imaging spectrometer for molecular fragmentation ...

The three-body fragmentation dynamics of triply charged allene (CH₂CCH₂³⁺) induced by 50-keV/u Ne⁸⁺ ion impact is studied by measuring the charged fragments in coincidence using the reaction...