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Photo-excited dynamics of CH_2N_2; time-dependent density functional theory HOSIK LEE, NEC Corp., YOSHIYUKI MIYAMOTO, NANO ELECTRONICS RESEARCH LABORATORIES, NEC CORPORATION TEAM, CREST, JAPAN SCIENCE AND TECHNOLOGY AGENCY TEAM — A highly reactive organic molecule carbene has been an important subject in organic chemistry in several decades. The carbene which is formulated by R_1R_2C : shows high yield and lesser or no side products during its reaction [1]. By using ultra-fast (sub-pico second) laser flash photolysis(LFP) technique to its precursor diazirine or diazomethane, the highly reactive short-living ($\sim$100 fs) carbene can be conveniently prepared and used for production. In this study, photo-excited dynamics of diazirine and diazomethane will be shown within the scheme of the first- principles time-dependent density functional calculations. With quite good agreements to experimental photo-excitation spectra, our preliminary calculation results show different phases of molecular motion which hardly is achieved with thermal effect. Temperature-induced kinetic effect in the phto-excited dynamics also is discussed.

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