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Quantum Chemistry based Coupled Electron Nuclei Dynamics Simulation TOMOTAKA KUNISADA, HIROSHI USHIYAMA, KOICHI YAMASHITA, The University of Tokyo — Electron dynamics with classical nuclei motion was performed to study electron-nuclei coupled (non-adiabatic) process of molecular system. Non-adiabatic transition from one adiabatic state from another adiabatic state occurred during the simulation, which was confirmed by monitoring adiabatic state populations. The change of charge distribution and dipole moment in the molecule was analyzed in order to study electron dynamics. To see electron dynamics more clearly, the change of the electronic character of the electron wave function was examined in terms of configuration functions. These results show that, not only the population of each adiabatic state but also the coherence between adiabatic states plays important roles in such ultrafast electron dynamics induced by non-adiabatic transition.

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