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Role of multiple orbital dynamics in multiphoton ionization of CO_2 in strong laser fields: The time-dependent Voronoi-cell finite difference method[1] SANG-KIL SON, SHIH-I CHU, University of Kansas — We theoretically investigate multiphoton ionization (MPI) of carbon dioxide in strong linearly-polarized laser pulses as a function of the angle between the molecular orientation and the field polarization. For a multicenter singularity problem in polyatomic molecules, we develop a new time-dependent Voronoi-cell finite difference (TDVFD) method with highly adaptive molecular grids. Many-electron time-dependent density functional calculations are performed by TDVFD, taking into account the detailed electronic structure and responses in multiple orbital dynamics. Our results show that the angular dependence of MPI is reflected by the perturbed orbital symmetry of multiple orbitals. The maximum peak of MPI is calculated at 40 degree in fair agreement with the recent experiment, which is significantly deviated from previous theories based on the single active electron approximation.

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