

Abstract Submitted
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Designing Laser Pulses to Control Molecular Motion QINGHUA REN, GABRIEL BALINT-KURTI, FREDERICK MANBY, School of Chemistry, University of Bristol, Bristol, BS8 1TS, UK, MAXIM ARTAMONOV, TAK-SAN HO, HERSCHEL RABITZ, Department of Chemistry, Princeton University, Princeton, New Jersey 08544 — A new method for incorporating polarization effects of the strong electric field into optimal control calculations is presented. An Electric-Nuclear Born-Oppenheimer approximation is introduced in which both the nuclear motion and the fluctuations of the external electric field are assumed to be slow compared with the speed at which the electronic wavefunction responds to these changes, which permits the generation of a potential energy surface that depends not only on the geometry of the nuclei, but also on the electric field strength and on the orientation of the molecule with respect to the electric field. As an illustration, it is firstly applied to the optimal control of the vibrational excitation of a hydrogen molecule aligned along with the field direction.^[1] And then it is extended to full three dimensions by allowing the H₂ molecules to rotate as well as vibrate.^[2] All calculation results show that it is possible to design shaped laser pulses that can excite H₂ either vibrationally, rotationally or both with a probability higher than 90%. ^[1] G. G. Balint-kurti, F. R. Manby, Q. Ren, M. Artamonov, T. Ho, and H. Rabitz, *J. Chem. Phys.* 122, 084110 (2005). ^[2] Q. Ren, G. G. Balint-kurti, F. R. Manby, M. Artamonov, T. Ho, and H. Rabitz, *J. Chem. Phys.* (in press).

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