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Ab initio design of laser pulses to control molecular motion GABRIEL BALINT-KURTI, QINGHUA REN, FREDERICK MANBY, University of Bristol, MAXIM ARTAMONOV, TAK-SAN HO, HERSCHEL RABITZ, University of Princeton, SHIYANG ZOU, University of Bristol, HARJINDER SINGH, IIIT Hyderabad, BRISTOL TEAM[1], PRINCETON TEAM[2] — Our recent attempts to design laser pulses entirely theoretically, in a quantitative and accurate manner, so as to fully understand the underlying mechanisms active in the control process will be outlined. We have developed a new Born-Oppenheimer like separation called the electric-nuclear Born-Oppenheimer (ENBO) approximation. In this approximation variations of both the nuclear geometry and of the external electric field are assumed to be slow compared with the speed at which the electronic degrees of freedom respond to these changes. This assumption permits the generation of a potential energy surface that depends not only on the relative geometry of the nuclei, but also on the electric field strength and on the orientation of the molecule with respect to the electric field. The range of validity of the ENBO approximation is discussed. Optimal control theory is used along with the ENBO approximation to design laser pulses for exciting vibrational and rotational motion in H_2 and CO molecules. Progress on other applications, including controlling photodissociation processes, isotope separation, stabilization of molecular Bose-Einstein condensates as well as applications to biological molecules also be presented. *Support acknowledged from EPSRC.

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