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Quantum simulations for analysis and control of reactions by laser pulses

Recent experiments demonstrate optimal control of competing chemical reactions by laser pulses. The optimal pulses contain information about the control mechanism. Decoding this information has been a challenge since the theoretical prediction and experimental discovery of optimal control by Rabitz et al and by Gerber et al, respectively. I shall demonstrate the successful decoding of an optimal laser pulse for selective photo-ionization of the organometalic compound, $CpMn(CO)_3$, without competing loss of the ligands (1). In a second part of the lecture, I shall demonstrate the design of infrared plus visible or ultraviolet laser pulses for the control of various processes, including the breaking of strong versus weak bonds in $BaFCH_3$ (2), symmetry breaking in FHF- (3), control of momenta for selective bond breaking in HOD (4), control of torsional angular momenta for ignition of a molecular rotor (5), and coherent spin control for FCl in an Ar Matrix, with 10 fs time resolution (6).
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Predavanje bo v angleščini, vljudno vabljeni!