CONTROL via ANALYSIS and INVERSION

Feedback control experiment to optimize CpMn(CO)₃²⁻ (vs. CpMn(CO)₂²⁻) Products produced in neutral or ion surfaces?

Pump-probe with optimal durations

Pump-probe mechanism

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Neutral-to-ionic transition dipole couplings

THEORY from first principles

Nonadiabatic couplings

Neutral-to-ionic transition dipole couplings

FUTURE

2d ab initio potential energy surfaces
2d non-adiabatic couplings
2d neutral-to-ionic transition dipole couplings

THEORY

Non-resonant multi-photon transitions (NMT), TP C3

TDSE for the resonant state space (projection operator technique):

Effective field Hamiltonian for a two photon transition:

Effective TDSE with respect to the resonant electronic states:

Non-ZEKE transitions, G. Paramonov (Minsk) & TP C6

 discretization of continuum
semiclassical, perturbation theory (weak field)

Non-ZEKE transitions, G. Paramonov (Minsk) & TP C6

time-dependent Koopmans’ picture (medium field)

Optimal control theory with NMT + non-ZEKE, TP C3

ANALYSIS and CONTROL

Control of competing ligand dissociation
Goal: Laser repairing of DNA mutation

Learning from simple: Cl-Ag-Br

to complex: Cytosine-Ag+ - Adenine (or Purine)