

Controlling Nuclear and Electronic Motion in Molecules

by

Harjinder Singh

in

Proceedings of Theory Conference on "Ten Years of Excellence in Science: 2006 - 2016"
(Theory Conference)

Report No: IIIT/TR/2017/-1



Centre for Computational Natural Sciences and Bioinformatics
International Institute of Information Technology
Hyderabad - 500 032, INDIA
January 2017

Controlling Nuclear and Electronic Motion in Molecules

Harjinder Singh

*International Institute of Information Technology Hyderabad (IIIT-H), Gachibowli,
Hyderabad, 500032, India*

Email: harjinder.singh@iiit.ac.in

Abstract

We will present our work on controlling nuclear and electronic motion in molecules using laser pulses designed using Optimal control theory (OCT). The control problem is formulated as the maximization of cost functional made of an objective function along with the constraints on the field fluence. The objective function has the prescribed dynamical goals. A detailed analysis of the optimal pulse reveals complex path-ways to arrive at seemingly simple goals. We have used OCT to obtain infrared laser pulses for the selective vibrational excitation of several different systems, from a simple diatomic to triatomic systems located in complex molecular environments. Controlled initiation of intramolecular H-transfer in malonaldehyde using ultrashort uv-laser pulses through an optically bright electronic excited state as a mediator will be discussed. Finally, our attempts to control the quantum dynamics of N-H photodissociation of pyrrole via a counterintuitive coupling of electronic states using uv-laser pulses will be discussed.

References:

- [1] K R Nandipati, H. Singh, S N Reddy, K A Kumar and S Mahapatra, *Eur.Phys.J., D 68 (2014) 255*
- [2] S Sharma, H Singh, GG Balint-Kurti, *J. Chem. Phys. 132, 064108 (2010)*