Abstract Submitted
for the DAMOP12 Meeting of
The American Physical Society

Optimal Control Bounds of Molecular Orientations in Finite Temperatures[1] SHENG-LUN LIAO, National Taiwan University, Taiwan, TAK-SAN HO, HERSCHEL RABITZ, Princeton University, SHIH-I CHU, University of Kansas — We investigated the optimal control bounds for the orientation of molecular systems in finite temperatures. The upper bounds of orientation controls are known to depend on both the temperature that determines the initial mixed states and the number of rotational states that can be excited by laser pulses. We considered the OCS molecule as an example to numerically demonstrate that a high degree of field-free-orientation can be achieved by optimally shaped pump fields in THz region [1]. To this end, we have implemented a fast monotonically convergent iterative procedure to obtain optimal orientation control pulses, by extending our recently formulated two-point boundary-value quantum control paradigm (TBQCP) for the pure-state optimal control problems [2-4] to the mixed-state ones. It was found that the degree of orientation could achieve 0.83 dynamically, which is 96% of the kinematical maximum, at T=100K.

[1] Sharly Fleischer, Yan Zhou, Robert W. Field, and Keith A. Nelson, Phys. Rev. Lett. 107, 163603 (2011).
[2] Tak-San Ho and Herschel Rabitz, Phys. Rev. E 82, 026703 (2010)
[3] Emanuel F. de Lima, Tak-San Ho, Herschel Rabitz, Chem. Phys. Lett. 501, 267 (2011).
[4] Sheng-Lun Liao, Tak-San Ho, Shih-I Chu, and Herschel Rabitz, Phys. Rev. A **84**, 031401 (2011).

[1]This work was partially supported by DOE and NSF and by MOE-NSC-NTU-Taiwan.

Sheng-Lun Liao
National Taiwan University

Date submitted: 26 Jan 2012 Electronic form version 1.4