# THE MOLECULAR GEOMETRIC PHASE AND LIGHT-INDUCED CONICAL INTERSECTIONS

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Potential energy surfaces for electronic states of molecules in strong electromagnetic fields can be described in the dressed-state formalism, which introduces light-induced potentials. A light-induced conical intersection (LICI) [1] appears when two electronic states intersect due to the presence of an external electric field and when the dipole coupling between the field and the molecule vanishes. There are several aspects of quantum dynamics near LICIs, which still require a thorough investigation. How do non-adiabatic effects manifest themselves in polyatomic molecules in strong electromagnetic fields? Are the natural conical-intersections (NCI) and the light-induced conical intersections identical in nature? Do topological effects (Berry phase) [2] influence the nuclear dynamics around NCIs and LICIs? To answer these questions, a computer code for time-propagation of the ro-vibronic wavefunction on multiple coupled potential energy surfaces has been developed. The time-independent zero-order basis is taken from the DUO suite [3], which solves the full ro-vibronic Schrödinger equation for diatomic molecules. Non-adiabatic nuclear dynamics near LICIs will be presented on the examples of NaH and CaF molecules, with a perspective for extension to polyatomics.

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[3] S. N. Yurchenko, L. Lodi, J. Tennyson, A. V. Stolyarov, Comput. Phys. Commun., 202, 262, 2016