

Time-dependent quantum dynamics of achiral and chiral molecules under coherent irradiation

We plan to employ and develop the GENIUSH program package [1] to investigate the time-dependent quantum dynamics of chiral and achiral polyatomic molecules under irradiation with coherent infrared radiation. So far relatively few prototypical systems have been studied and we plan to investigate among other systems the full-dimensional tunneling dynamics in simple achiral ammonia isotopomers and the chiral NHDT variant for which global full-dimensional potential energy and electric dipole moment hypersurfaces are available in Zurich [2,3]. We shall continue and complete work which has already been made in part before and make systematic comparisons between full-dimensional and approximate reduced-dimensional results using the quasiadiabatic channel reaction path Hamiltonian approximation and other approximate lower dimensional calculations. From these studies we shall try to learn how to optimize approximate calculations on higher dimensional problems. We also plan to extend and complete investigations of coherent excitation of phenol isotopomers [4,5] and of fluoroform [6].

The project is of general fundamental relevance [2,7] and has in addition importance for ongoing time-dependent experiments aiming at the detection of molecular parity violation [7-12] and also experiments on ammonia with hyperfine resolution [10].

References

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