

## Detailed work plan of the STSM

### Time dependent quantum dynamics of polyatomic molecules and clusters under coherent irradiation using URIMIR and related packages

17.4.2017-25.4.2017: We plan to investigate the time dependent quantum dynamics of chiral and achiral polyatomic molecules and clusters under irradiation with coherent infrared radiation using the URIMIR package and related codes. So far relatively few prototypical systems have been studied and we plan to investigate among other systems the simple achiral hydrogen bonded dimer (HF)<sub>2</sub> and the chiral molecule hydrogen peroxide HOOH for which full-dimensional potential and electric hypersurfaces are available in Zurich. We shall 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 investigations using light of different polarizations for excitation of a prototypical atomic system such as Iodine including hyperfine structure with the aim of future simulations of molecular systems including hyperfine structure.

The project is of general fundamental relevance [1,2] and has in addition importance for ongoing time dependent experiments aiming at the detection of molecular parity violation [3-6].

#### References

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