Scientific report on the STSM entitled

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

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The Short-term Scientific Mission (STSM) of Ioannis Thanopulos entitled "Time dependent quantum dynamics of polyatomic molecules and clusters under coherent irradiation using URIMIR and related packages" took place during 17.4.2017-25.4.2017 in the group of Prof. Martin Quack at the ETH Zurich. The goal of the mission has been the investigation of the time dependent quantum dynamics of polyatomic molecules and clusters under coherent irradiation using the URIMIR package, as well as other related software developed in the group of Prof. Martin Quack.
Towards this end the following tasks have been initiated:

1. The absorption spectrum of the infrared magnetic dipole induced transition in the ground term of the atomic iodine under irradiation of a strong laser field at off-resonant conditions within the Floquet approximation [1] is investigated using the URIMIR package [2,3]. As a starting project the spectroscopic data of the iodine atom under radiation-free conditions used in these calculations are obtained by *ab initio* calculations using a multi-configurational Hartree-Fock atomic structure package for large scale calculations [4]. The preliminary results of these calculations are in good agreement with results from atomic iodine spectroscopic experiments obtained in the Quack group [5]. We have started the study of coherent transitions under various conditions with the aim of better understanding the dynamics of radiative transitions in the iodine atom as a prototypical system for magnetic dipole dominated transitions, important, for instance, for the iodine laser but also in special experiments with laser detection of iodine atoms.

2. The infrared multiphoton excitation of the H_2O_2 molecule along the torsional mode is investigated using the URIMIR package. For this purpose, the vibrational spectrum of the hydrogen peroxide is calculated using a full-dimensional global analytical potential surface [6]. More specifically, the vibrational eigenstates are obtained by two methods: (i) full-dimensional variational calculations [7,8], and (ii) with the Quasiadiabatic Channel Reaction Path Hamiltonian [7,8,9,10], a modified version of the RPH approach [11]. Software developed in the group at

ETH Zurich is used. The electric dipole transition moments between torsional levels are calculated *ab initio* approximately. The quantum dynamics of the hydrogen peroxide is further investigated during and after infrared multiphoton excitation along the torsional motion within the weak-field quasiresonant approximation [1] as implemented in the URIMIR package. The work is being extended to clusters.

The STSM overlapped in time partially with the *International Workshop on Molecular Quantum Dynamics and Kinetics* organized during 18.4.2017-20.4.2017 at the ETH Zurich by the working group "Time-Resolved Method Developments" of the COST Molim Action, where Ioannis Thanopulos also gave an invited lecture. The interaction with the workshop participants has contributed positively to the scientific value of the STSM.

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