

# Quantum Dynamics Model as an Approach to Study Atomic and Molecular Structures

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**Abstract**— This work is very necessary to find field of applications for our theories concerning the quantum dynamics applying for atomic and molecular structure. On the recent years, study of atoms and molecules and its structures gets an extremely attentions of tasks of many researchers institute, specially, the photodissociation processes, which needs a variety of computational chemistry, in the two areas, molecular mechanics and electronic structure theory. Also, we need a different computer programs to calculate the total energy absorption cross-section for the photodissociation processes of a molecules, using quantum dynamical methods, which will be one of my main tasks on this research review article. There are two major classes of electronic structure methods: Semi-empirical methods and ab initio methods. The two classes are of interest for both theoreticians and experimentalists.

Quantum dynamics is an approach to study atomic and molecular Structures. This work deals with the computational method used in quantum dynamics approach and so developing theoretical techniques and computer programs concerning the quantum dynamics applying for atomic and molecular structure.

**Keywords;** Quantum Dynamics méthodes, photodissociation processes.

## I.. INTRODUCTION

We call *molecular dynamics* (MD) a computer simulation technique where the time evolution of a set of interacting atoms is followed by integrating their equations of motion. In molecular dynamics we follow the laws of classical mechanics, and most notably Newton's law:  $\mathbf{F}_i = \mathbf{m}_i \mathbf{a}_i$  for each atom  $i$  in a system constituted by  $N$  atoms. Here,  $\mathbf{m}_i$  is the atom mass,  $\mathbf{a}_i$  its acceleration, and  $\mathbf{F}_i$  the force acting upon it, due to the interactions with other atoms. Therefore, in contrast with the Monte Carlo method, molecular dynamics is a deterministic technique: given an initial set of positions and velocities, the subsequent time evolution is in principle completely determined. In more pictorial terms, atoms will "move" into the computer, bumping into each other, wandering around (if the system is fluid), oscillating in waves in concert with their neighbors, perhaps evaporating away from the system if there is a free surface, and so on, in a way pretty similar to what atoms in a real substance would do. The computer calculates a trajectory in a  $6N$ -dimensional phase space ( $3N$  positions and  $3N$  momenta). However, such trajectory is usually not particularly relevant by itself.

Molecular dynamics is a statistical mechanics method. Like Monte Carlo, it is a way to obtain a set of configurations distributed according to some statistical distribution function, or statistical ensemble. An example is

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the microcanonical ensemble, corresponding to a probability density in phase space where the total energy is a constant  $E$ :  $\delta(H(\Gamma) - E)$ . Here,  $H(\Gamma)$ , is the Hamiltonian, and  $\Gamma$  represents the set of positions and momenta.  $\delta$  is the Dirac function, selecting out only those states which have a specific energy  $E$ . Another example is the canonical ensemble, where the temperature  $T$  is constant and the probability density is the Boltzmann function  $\exp(-H(\Gamma) / k_B T)$ .

According to statistical physics, physical quantities are represented by averages over configurations distributed according to a certain statistical ensemble. A trajectory obtained by molecular dynamics provides such a set of configurations. Therefore, a measurements of a physical quantity by simulation is simply obtained as an arithmetic average of the various instantaneous values assumed by that quantity during the MD run.

Statistical physics is the link between the microscopic behavior and thermodynamics. In the limit of very long simulation times, one could expect the phase space to be fully sampled, and in that limit this averaging process would yield the thermodynamic properties. In practice, the runs are always of finite length, and one should exert caution to estimate when the sampling may be good ("system at equilibrium") or not. In this way, MD simulations can be used to measure thermodynamic properties and therefore evaluate, say, the phase diagram of a specific material.

Beyond this "traditional" use, MD is nowadays also used for other purposes, such as studies of non-equilibrium processes, as an efficient tool for optimization of structures overcoming local energy minima (*simulated annealing*), properties of materials and other applications.

All chemical and biological processes are determined by interactions between molecules. By understanding these interactions on the most basic level progress can be made in a fundamental understanding of 'real world' systems. Basic means specification of all internal states of the molecule (rotation, vibration,.....etc.) and of the collision (velocity, orientations, impact distances,....) before, during, and after a single collision event. Studies of this type are the most challenging in chemical physics and very few systems have been investigated in the required detail thus far.

Our article deals with theoretical and computational aspects of molecular and material sciences, with emphasis on the unified treatment of physical and chemical kinetics using Quantum Molecular Dynamics (QMD). It includes collision-induced and photon induced phenomena in the gas

phase, clusters, and at solid surfaces. The aim is to provide a fundamental approach to molecular dynamics, where electronic and nuclear motions are consistently coupled to account for quantal effects. We will use quantum and statistical mechanics, mathematical, and computational methods, to describe time-dependent phenomena (such as femtosecond dynamics and spectra) in both simple and complex molecular systems.

*Abdel-hafiez A., et.al.*, International Journal of the Physical Sciences Vol. 5(7), pp. 978-983, July 2010. We have theoretically studied the nonadiabatic transitions among the lower states with  $W = 1u$  symmetry { $1u$  (Lindeman and Wiesenfeld, 1979) to  $1u$  (Alexander et al., 2000)} in the photodissociation of  $Br_2$  using the complete active space self-consistent field (CASSCF) computations and the time-independent Schrodinger equations. The CASSCF wave function is formed from a complete distribution of a number of active electrons in a set of active orbitals, which in general constitute a subset of the total occupied space. From the configuration analysis of the CASSCF wave functions, we found that the non adiabatic transition between  $1u$  (Bracker et al., 1999) and  $1u$  (Lindeman and Wiesenfeld, 1979) is a non crossing type, while that between  $1u$  (Bracker et al., 1999) and  $B3P0+u$  is a crossing type. The spectroscopic constants for the  $X1Sg +$ ,  $A3P1u$  and  $B3P0+u$  states of  $Br_2$  have been calculated. The absorption cross section for the ground and the lower excited states in the photodissociation of  $Br_2$  molecule has been presented as well as the numerical estimates of nonadiabatic transition probabilities. Also, the five highest occupied and the five lowest unoccupied orbitals of  $Br_2$  have been calculated [1-4]. *Dongfang Zhang, et.al.*, *Chemical Physics* 342 (2007) 119–125. The photodissociation dynamics of  $HI$  molecule has been studied within the A band range. Partial and total extinction cross-sections are obtained from numerical calculations. The frequency dependent branching fraction is determined and agrees with the experiment. The curve-crossing probabilities are derived resorting to the anisotropy data of fragmentation product and the one-dimensional Landau–Zener model is used to examine the possibility that non adiabatic mechanism occurs in the dissociation process. The results suggest that the contribution of non adiabatic mechanism to  $HI$  photofragmentation, which may be caused by spin–rotational coupling, is not significant over the low energy part of the A band and thus can be ignored, although the angular distribution is less anisotropic in this energy regime [5-9]. *Dongfang Zhang, et.al.*, *Chemical Physics Letters* 428 (2006) 49–54. The dissociation processes of  $Cl_2$  molecule have been studied at numerous photolysis wavelengths (310–470 nm) using time-dependent wave packet method. The initial wave packets are propagated on the excited state potentials utilizing the splitting operator technique. The optical cross-sections are calculated numerically by extracting the dynamics information at a

large internuclear separation. Applying the Rozen–Zener–Demkov model, the radial non-adiabatic transition probabilities from C1Pu to 1u(III) electronic state are predicted, the branching ratio of various product channels and anisotropy parameter  $b(Cl^*)$  are determined[10-13].

The molecular dynamics method was first introduced by Alder and Wainwright in the late 1950's (Alder and Wainwright, 1957,1959) to study the interactions of hard spheres. Many important insights concerning the behavior of simple liquids emerged from their studies. The next major advance was in 1964, when Rahman carried out the first simulation using a realistic potential for liquid argon (Rahman, 1964). The first molecular dynamics simulation of a realistic system was done by Rahman and Stillinger in their simulation of liquid water in 1974 (Stillinger and Rahman, 1974)[14-16].

The main targets of that article, is studying the molecular structure on the frame of both of Quantum chemistry and quantum dynamics. That studies allows us to study the motions of the nuclei and the electrons in molecules during chemical reactions (as shown on the Figure 1), and also, support the interpretation of experimental studies of photodissociation and other reactive processes, as well as localization of molecular orbitals In quantum chemistry, studying of the electronic motion of the molecules is of interest, and in quantum dynamics studying of the nuclear motion of the molecules is of interest.

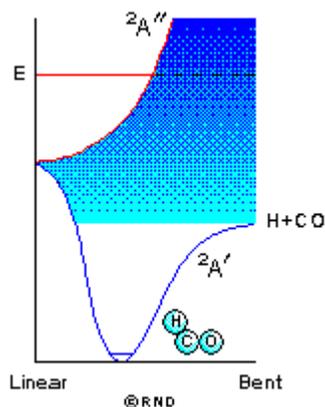


Fig.1. Model of the motions of the nuclei and the electrons in molecules during chemical reactions

Quantum Dynamics of atoms allow one to study and do calculations for molecular structures and molecular photodissociation dynamics, this can be in exploring the applicability of multiconfiguration of the time-dependent Hartree approximation in photodissociation dynamics. So that we need to have the following characteristics:

### First stage

- Electronic structure modeling to investigate and predicting many properties of molecules and reactions: Energies and structures of transition states, Thermochemical properties, Vibrational frequencies.
- Study of the Potential Energy Surface, which play an important role on studying the geometry optimizations of the molecules
- The treatments for molecular dynamics usually involve solutions of the time-dependent Schrodinger equations.
- The initial wave packets transfer into matrix representations
- Using time-dependent wave packet calculations on the compute of potential energy curves for the ground excited states.
- Numerical solutions for time-dependent Schrodinger equation using matrix representation for the fundamental set of equation of motion, we can creat different characteristics and comparing with different software like Gaussian, Colby
- Speed, angular and energy distributions of atoms can be comuted.
- Density Functional theory, Hartree-Fock theory and Perturbation theory will apply to predict molecular optimized structure parameters.
- Software like Gaussian and Colby, can serve as a powerful tool for exploring areas of chemical interest like potential energy surface and excitation energies.

### Second stage ( Study of the photodissociation dynamics)

- Wave-Packet dynamics within the multiconfiguration Hartree.
- Numerical and convergence studies within the multiconfiguration Hartree approach.
- Reactive scattering and Quantum dynamics within the multiconfiguration time-dependent Hartree approximation.
- Quantum dynamics simulation of the vibrational predissociation of the molecules.
- Study of the reaction cross sections via wave packet propagation study.

For the two –stages, I need deeply to cooperate with both theoreticians and experimentalists people who are interested in that active field.

### Third stage (The quantal motion of the nuclei of a molecule)

We will try to use quantum molecular dynamics, in which the algorithm for solving the time-dependent Schrodinger equation for distinguishable particles is use. It is usually applied to study the quantal motion of the nuclei of a molecule (quantum molecular dynamics).

The most characteristics of this algorithm, its a very powerful algorithm for propagating wave packets in several

(distinguishable) dimensions, but on the same time its a very complicated algorithm. From these characteristics:

- Configurations in a time-dependent Hartree treatment of the photodissociation of molecules.
- Quantum dynamics within the time-dependent Hartree approximation.
- Wave packet propagation for large molecular systems.
- Quantum dynamics of molecular reaction.
- Calculation of the reaction probabilities.
- Photodissociation of the complex molecules.
- Quantum dynamical wave packet calculations of molecules on surfaces.

For the first and second stages, characteristics will be study on the frame of the quantum chemistry approaches, but for the third stage, characteristics will be study in the frame of the quantum dynamics approach.

## II. METHODS OF STUDYING CHARACTERISTICS OF THE PHOTODISSOCIATIONS PROCESS

### II.1 QUANTUM MOLECULAR DYNAMICS (QMD)

1. Energy transfer, electron transfer and reactions in gas phase molecular collisions.
2. Energy transfer, electron transfer and reactions of molecules at solid surfaces.
3. Intermolecular forces in ground and excited electronic states.
4. Spectra and dynamics in atomic clusters.
5. Photodissociation of polyatomic molecules.
6. Light emission in collisions of ions with atoms and solid surfaces.

### II.2 THEORETICAL METHODS

1. Time-dependent many-electron theory; time-dependent molecular orbital and time-dependent Hartree-Fock approaches to molecular phenomena.
2. Few-body and many-body theory of molecular collisions; collisional time-correlation approach to many-atom collisions.
3. Statistical mechanics of response and rate processes.
4. Density matrix theory of relaxation, dissipation and fluctuations in extended molecular systems.

### II.3 COMPUTATIONAL METHODS

1. Numerical methods for the solution of differential

and integral equations of scattering.

2. Vibrational methods for scattering and time-dependent states.
3. Path integral and wave packet propagation in quantum dynamics.
4. Operator algebra methods for solving operator differential equations.
5. Numerical methods for the solution of the Liouville-von Neumann differential equation for the density operator.
6. Integration of stochastic differential equations for coupled quantal and classical degree of freedom, and of the generalized Langevin equations.
7. Integration of differential equations for coupled fast and slow degrees of freedom. The "relax-and-drive" method.
8. Calculation of molecular one-and-two-electron integrals for travelling atomic basis functions.

### II.4 COMPUTER VISUALIZATION AND ANIMATION OF MOLECULAR INTERACTIONS

1. Animation of the temporal evolution of both nuclear motions and electronic densities using nuclear trajectories and isocontours of electronic densities.
2. Animation of electronic transition and electron transfer obtained from time-dependent molecular orbitals.
3. Animation of light emission in collisions of ions involving electronic rearrangement and the related transient dipoles.  
. The spectra were recorded in 512 channels.

## III. ALGORITHM OF THE NUMERICAL TECHNIQUES

The algorithm depends on the numerical integration of the time-dependent Schrödinger equation [16].

$$i\hbar \frac{\partial \Phi(r,t)}{\partial t} = \hat{H}(r) \Phi(r,t) = \left[ \frac{-\hbar^2}{2m} \frac{d^2}{dr^2} + V(r) \right] \Phi(r,t)$$

where  $r$  is the bond distance,  $m$  the reduced mass of the molecule,  $V(r)$  the adiabatic potential energy, and  $\Phi(r, t)$  is the time-dependent wave function. The initial wave packets  $\Phi_n(r, t)$  is prepared by means of the ground state vibrational

wave function  $\Psi(r)$  times the appropriate transition dipole functions [7].

$$\Phi_n(r, t=0) = M_n(r) \Psi(r)$$

where  $\Phi_n(r, t=0)$  denotes the wave packet associated with the  $n$ th excited state,  $M_n(r)$  is the associated transition moment. Wave packet propagation using split operator (time step is  $\Delta\delta$ ) scheme

$$\Phi(r, t + \Delta\delta) = e^{-i\hat{T}\Delta\delta/2\hbar} e^{-iV\Delta\delta/\hbar} e^{-i\hat{T}\Delta\delta/2\hbar} \times \Phi(r, t)$$

The dynamics is probed at an analysis line fixed at a large value of  $r = r_\infty$ . Energy dependent amplitudes  $B_n(r_\infty, E)$  are obtained by Fourier transformation [15].

$$B_n(r_\infty, E) = \frac{1}{2\pi\hbar} \int_0^\infty \Phi_n(r_\infty, t) \exp[i(E - \hbar\omega)t/\hbar] dt$$

where  $E_0$  is the energy of origin transition,  $\hbar\omega$  denotes the incident energy. The partial cross-sections are obtained by

Table 1: The input parameters to perform the time-dependent wave packet calculation

Variable	Description	Value
Atomic masses	$\mu_H$	1.0079 amu
Reduced masses.	$\mu_1$	126.9045 amu
	$\mu$	1823.02 a.mu.
Range of grid	$r_{\min}, r_{\max}$	2.363–14.952 $a_0$
Number of grid points		2048
Position of $r_\infty$	$\Delta\delta$	9.452 $a_0$
Time step		0.483776 fs
Number of time steps	$r_{\text{abs}}$	8192
Start of absorbing region	$J_{\text{opt}}$	9.952 $a_0$
Amortization factor		0.15 <sup>-1</sup>

$$\sigma_n(\nu) = \frac{32\pi^2 k_n}{3c\epsilon_0} |B_n(r_\infty, E)|^2$$

where  $k_n$  is the asymptotic wave vector for the  $n$ th channel. The total cross-section amounts to the sum of the partial cross section,

$$\sigma_{\text{tot}}(\nu) = \sum_{n=1}^4 F_n \sigma_n(\nu)$$

where  $F_n$  is a degeneracy factor of the upper dissociative state. In order to get rid of the spurious recurrences at small grids, wave packets must be dissipated by the absorbing potential in the asymptotic domain. The coefficients of absorbing potential are  $J_{\text{abs}}(r) = 1.0$ ,  $r < r_{\text{abs}}$

$$J_{\text{abs}}(r) = \exp(J_{\text{opt}} \Delta\delta) \left( \frac{r - r_{\text{abs}}}{r_{\text{max}} - r_{\text{abs}}} \right)^{1.5}, \quad r_{\text{abs}} < r < r_{\text{max}}$$

where  $r_{\text{abs}}$  is the incipient point of damping and  $J_{\text{opt}}$  is a factor to modulate damping force. A compilation for all sorts of parameters is outlined in Table 1.

#### IV. TEST OF THE ALGORITHM AS A RESULT

In Fig.2 the Calculated  $I^*$  branching fractions (solid line) in comparison with experimental results: open circles – Gendron and Hepburn [17], open squares – Manzhos et al. [5], filled diamonds – Langford et al. [18], round dot – Schmiedl et al. [19], open triangle – van Veen et al. [20], gradient symbols – Brewer et al. [21–23]. The quantum yield  $\Phi_{I^*}[\lambda]$  for the spin-orbit excited state iodine in experiment is a fundamental characteristic and is usually dictated as

$$\phi_{I^*}[\lambda] = \frac{(I^*)}{(I) + (I^*)},$$

where  $(I)$  and  $(I^*)$  are concentrations of the  $I$  and  $I^*$  atoms resulting from the fragmentation reaction at a particular wavelength  $\lambda$ .

In fig. 3. the potential energy curves for low-lying states of HI is calculated. Restricted by the electric-dipole-forbidden and selection rules, the pertinent excited state potential curves that initially populated in the near ultraviolet region of the spectrum are four  $\Lambda$ -S molecular states, as shown in Fig. 3.

In fig. 4. Intensity profile of the partial and total absorption spectrum for a part of the A band is calculated, where Solid line – calculated,  $\diamond$  experimental data. As displayed in Fig. 4, the frequency dependent extinction cross-sections of separate electronic state along with their total cross-section is superimposed on the data of Ogilvie [24] in the same path length.

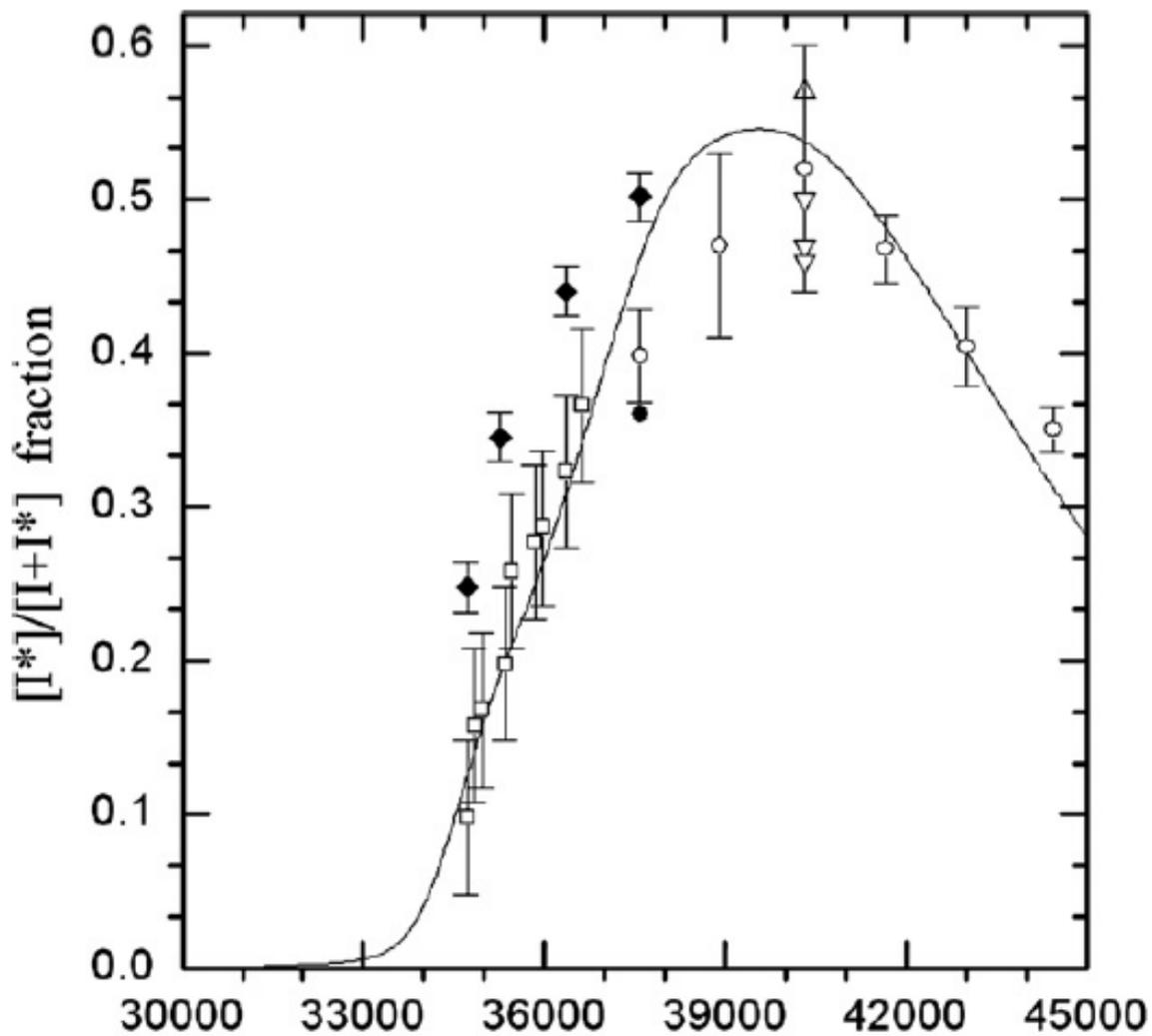


Fig.2. Photolysis energy/ cm<sup>-1</sup>

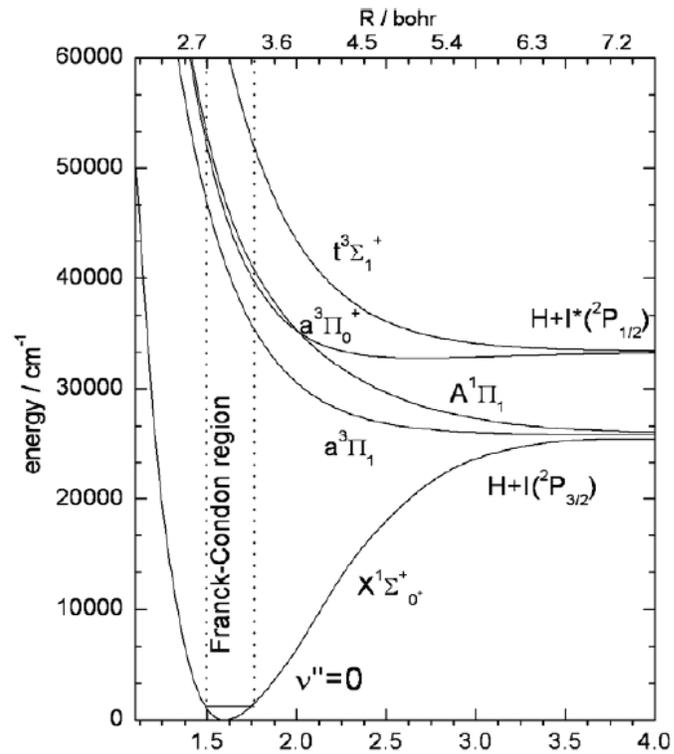


Fig.3. Interatomic Distance / Å

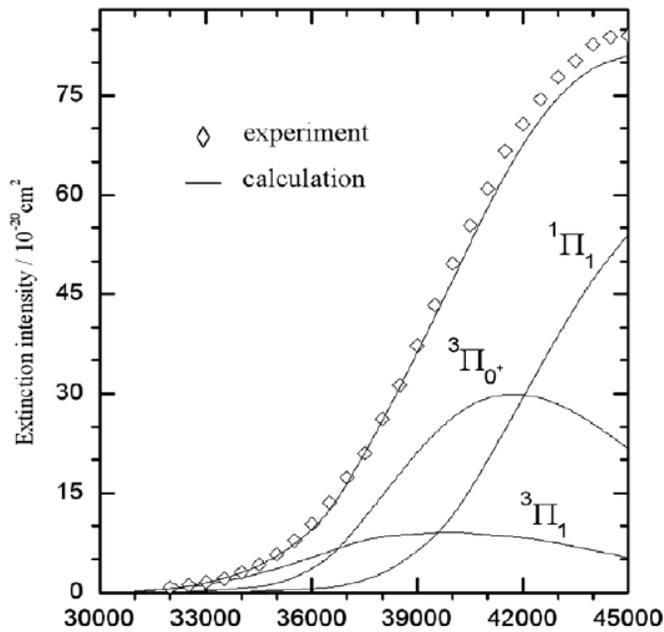


Fig.4. Transition frequency  $\nu$  ( $\text{cm}^{-1}$ )

### Field of applications of that research

- 1- Biological applications
- 2- Chemical and physical applications
- 3- Material science applications

#### 1)Used Software for the calculation

- Applications programs, Mat lab, Mathcad and Mathematica.

For calculus, data analysis, some special plots and graphics

- Software C++. For solving all algorithms.
- Origin software for Graphics, some data analysis.
- Gaussian03 and Gaussian view.

### V. CONCLUSIONS

As a test, the dissociation processes of hydrogen iodide have been investigated in detail. The extinction cross-sections and final product state population are obtained by the time dependent calculations, which exhibit a good agreement with the previous experimental results. Based on the observed anisotropy parameter, the crossing behavior is simulated by using the Landau-Zener model and is not accurately reproduce the angular distribution change as a function of dissociation wavelength, indicates that photolysis proceeds without salient nonadiabatic mechanism between the  $a^3P_0^+$  and  $A^1P_1$  potentials and nonadiabatic curve-crossing is of minor importance in the dissociation after excitation at the low energy end of the A band.

Study of different characteristics concerning molecular electronic structures, properties of materials, and optical properties, need on equal

foot both of experimental and theoretical views, what it need work team.

Both of quantum chemistry and quantum dynamics are study the molecules, but the characteristics which can be created by quantum chemistry is quiet different from those create by the quantum dynamics. That mean that we may could to create bridge between both to create both of characteristics.

The development and application of theoretical (computational) methods that can be used in studying properties of materials. The methods are based on the application of quantum theory. Such study of the materials is of interest range from molecules, via clusters and polymers, to solids, and on structural, electronic, and optical properties.

By this way, more extensions and developing of Molecular Dynamics with or without quantum treatments can be make. Also, several chemical physics problem can be solve, what it make a collaboration between us will be more than the sum of each of us separately.

The following general characteristics could be determined:

- 1- viewing molecular structures and animating molecular trajectories.
- 2- A utility for animating molecular vibrations.
- 3- The display of molecules.
- 4- Configuration for graphical representation of molecule.
- 5- Analyzing, and manipulating the three-dimensional structure of biological macromolecules,
- 6- Generating high quality images of molecules.
- 7- 3D viewer for molecular charge distributions.
- 8- Create a bridge between most of the molecular software packages.

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