Ionization of water molecules in liquid and gaseous phases by electron impact

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INTRODUCTION & AIM

Water molecules ionization is an important reaction in domains such as plasma physics, fusion experiments, astrophysics, and in the study of ionizing collisions on living matter. Moreover, secondary slow electrons (products of the ionization) are of importance in the mechanisms that lead to cell alteration [1]. So, the study of the ionization of liquid water molecules by electron impact is mandatory, for example, for medical researches in the field of Radiobiology.

A first order model is employed (see previous works [2-4]) to calculate triple differentials cross sections for the ionization of water molecules in the liquid and gaseous phases by energetic incident electrons. Asymmetric collisions in a coplanar geometry are considered. The condensed phase is described through a formalism based on the Wannier orbitals, while the gas by Gaussian functions. Comparison with the vapor phase are in a good qualitative agreement with our calculations and show the trend of different phases.

METHOD

In the framework of an independent electron model, eight-fold Differential Cross Sections for single ionization of the active electron, at a fixed molecule orientation, are obtained as,

$$\sigma^{(8)}(\alpha,\beta,\gamma)=\frac{d\sigma}{dE_e\,d\Omega_e\,d\Omega_s\,d\Omega_{mol}}=N(2\pi)^4\frac{k_s k_e}{k_i}\left|\left\langle \Psi_f^-\left|V_i\right|\psi_i\right\rangle\right|^2$$

➢ k_i, k_s and k_e are the incident, scattered and ejected electron momenta, respectively
➢ $d\Omega_{mol}=sen\beta\,d\alpha\,d\beta\,d\gamma$ where α, β, γ are the Euler angles
➢ V_i is the perturbation in the initial channel $\quad V_i=\frac{1}{|\vec{r}-\vec{R}|}-\frac{1}{R}$
➢ ψ_i and Ψ_f^- are the initial and the final wavefunctions (the latter with correct boundary conditions), respectively

$$\psi_i=\frac{e^{i\vec{k}_i\cdot\vec{R}}}{(2\pi)^{3/2}}\Phi(\vec{r})\qquad \Psi_f^-\approx\frac{e^{i\vec{k}_s\cdot\vec{R}}}{(2\pi)^{3/2}}C(v,k_e;\vec{r})$$

C is a Coulomb wave function

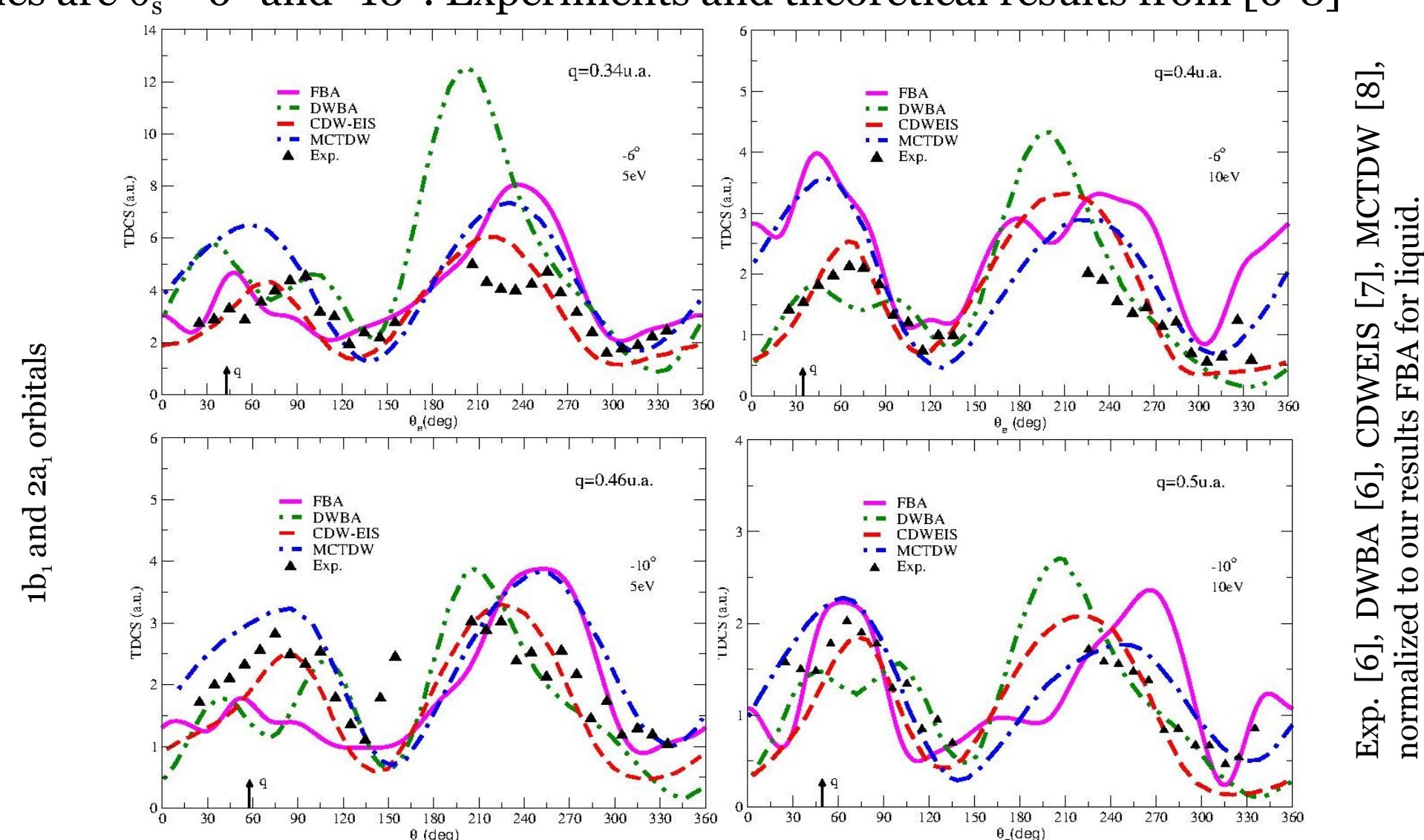Φ(r) : initial molecular orbital obtained through a Wannier formalism[5] for the liquid and for the gas from Gaussian functions centered in each atom of the molecule.

Effective molecular orbitals for liquid

1B₁   2A₁   1B₂   1A₁
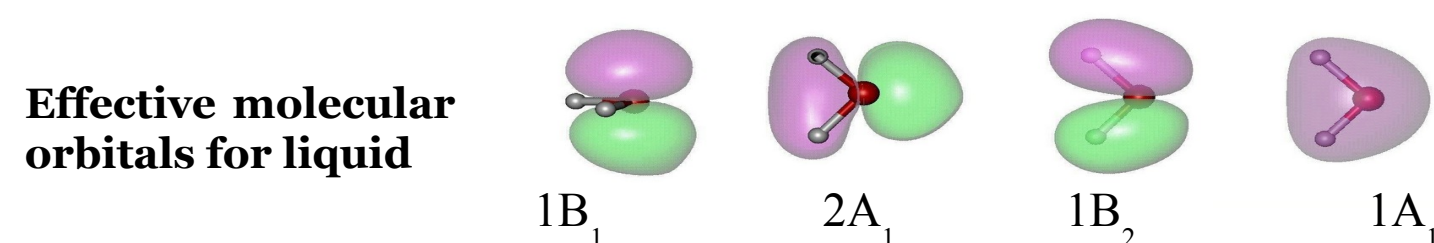
Integrating over de Euler angles we obtain five-fold Differential Cross Sections averaged over all the possible molecular orientations. They reduce to Triple Differential Cross Sections (TDCS) in a coplanar geometry, where the ejected electron is contained in the collision plane defined by the incident and the scattering directions. TDCS describe the angular distribution of the ejected electrons at a given ejection energy E_e from each orbital of the liquid water molecule. The momenta of the incident and scattered electrons are fixed.

RESULTS & DISCUSSION

We present TDCS (only contributions of the two most external orbitals) for ionization of water molecules as a function of the ejection angle θ_e. The incident energy is $E_i=81eV$ and the ejection energy is $E_e=5eV$ and $10eV$ while scattering angles are $\theta_s=-6°$ and $-10°$. Experiments and theoretical results from [6-8]

1b₁ and 2a₁ orbitals

Exp. [6], DWBA [6], CDWEIS [7], MCTDW [8], normalized to our results FBA for liquid.

Under the given kinematic conditions for both theoretical and experimental results, the characteristic double-lobe structure of the binary region—typical of p-type orbitals—does not appear; instead, a single peak is observed (with the exception of the DWBA).

1b₁ orbital

Exp. [6], CDWEIS [7], MCTDW [8], normalized to our results.
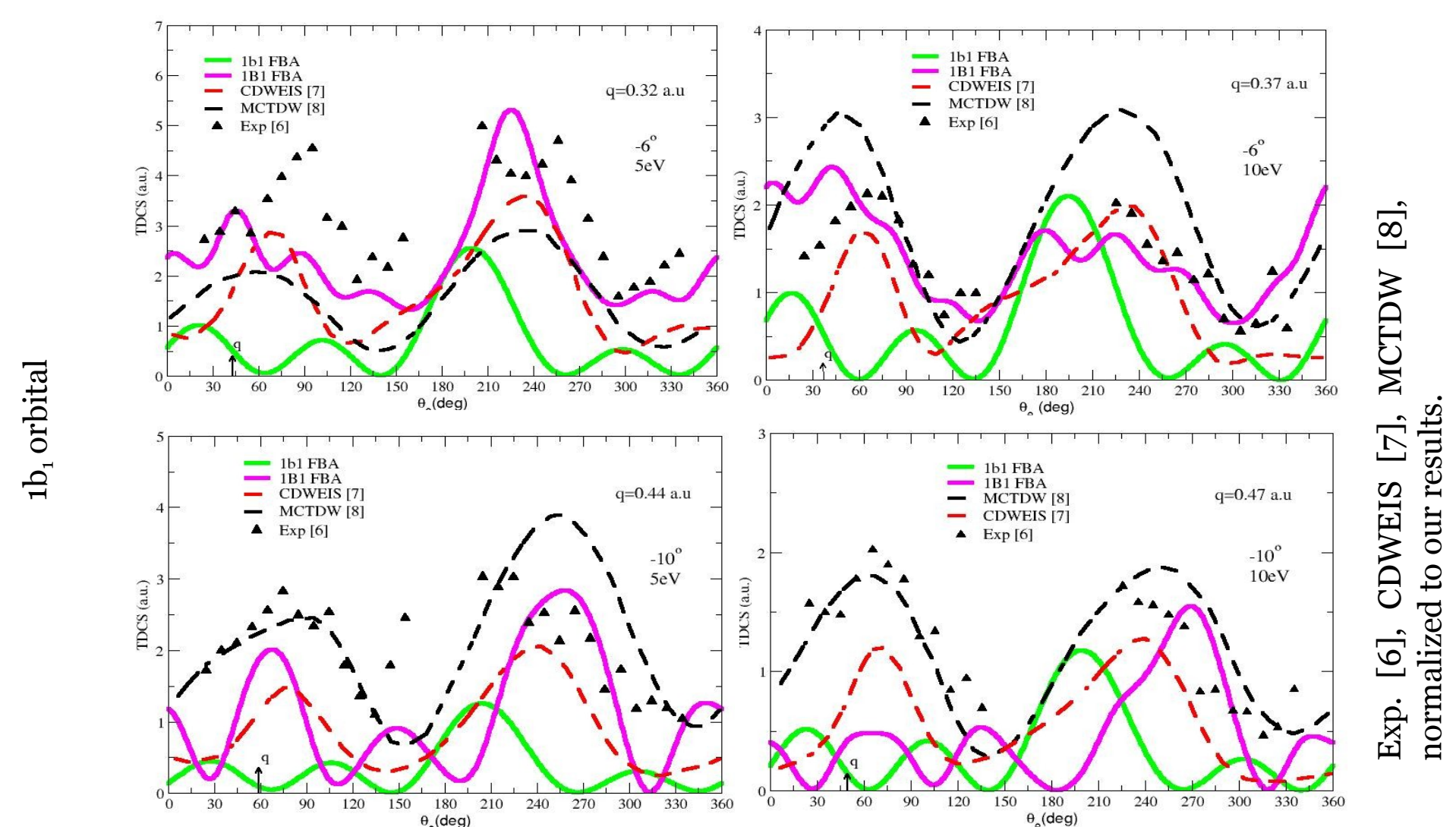
We find qualitative agreement with our predictions for both phases. The results reproduce the structures of the experimental gas-phase TDCS [6], showing the characteristic binary and recoil regions.

At lower ejection energies, the ratio between the magnitudes of the maxima in both regions becomes more significant, with the recoil peak being dominant; this trend is also observed in the theoretical data for the gas phase.

CONCLUSION

Our TDCS exhibit the primary physical features observed in the experimental data for vapor, specifically the binary and recoil regions. A comparison of our calculations for the liquid and gas phases with existing predictions and experimental data for the gas phase shows qualitative agreement. The results successfully reproduced the characteristic binary and recoil regions. Under the kinematic conditions, for summed contributions, a single peak in the binary region is found in accordance with Ren et al [6]. At this low incident energy (81 eV), the TDCS are qualitatively well described by the FBA. In the summed contributions, the ratio between the binary and recoil maxima changes as E_e increases, a trend also reproduced by our results. For the most external orbital our cross sections of the gas are smaller than those for the liquid, primarily in the binary region.

FUTURE WORK / REFERENCES

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