EIPAM Sientific Report of Exchange grant Ref.891

Grantee:
Dr. Bratislav Marinkovic, Institute of Physics, Centre for Atomic and Subatomic Physics, Laboratory for Atomic Collision Processes (ACP), 11080 Belgrade-Zemun, P.O. Box 68, Pregrevica 118, Serbia

Host researcher:
Dr. Gustavo Garcia, Instituto de Matematicas y Fisica Fundamental, CSIC, Serrano 113-bis, 28006 Madrid, Spain

Approved duration of the exchange grant:
3 weeks

Purpose of the visit

The purpose of the visit was twofold: a) establishing the collaboration of two groups and introducing different experience in experimental methods accumulated in both groups; b) joint work on the same targets chosen for the investigations in lines of the EIPAM mission.

Description of the work carried out during the visit

During the visit the work was carried out very intensively on several objectives. One activity was involved in obtaining the new calculations of electron interactions with amino acids, specifically glycine and alanine. The amino acid molecules are of special interest since they are the essential molecular components of living organisms on Earth. Calculations of molecular cross sections are based on a corrected form of the independent-atom method (IAM), known as the SCAR (Screen Corrected Additivity Rule) procedure. In the standard IAM approximation the electron-molecule collision is reduced to the problem of collision with individual atoms by assuming that each atom of the molecule scatters independently and that redistribution of atomic electrons due to the molecular binding is unimportant.

Another activity was to process the raw data obtained from the experimental investigation of electron collisions by bio-molecular targets such as glycine and alanine. In order to convert the raw data of angular distributions of scattered electrons into relative cross section data, one needs to apply the effective path length correction factors. These factors depend on the kind of molecular target under investigation, geometry applied in the experiment, flow conditions of the effusive beam, and the steepness of differential cross sections (DCS) obtained.

Also, the comparison between experimental data and calculated values was done. Since the shape of differential cross sections agreed very well in all scattering angles except very small ones, normalization of experimental data points was done on the calculated absolute value at the scattering angle of 80 degrees. Extrapolation of measured data toward zero and 180^{o} scattering angles was done in such manner that the experimental integrated cross section matches calculated integral cross section.

Finally, the work was done on installation of a new experimental set-up for measuring the partial ionization cross sections. The apparatus is under preparation and the assembling of the main parts such as electron gun, time of flight tube, electron and ion detectors are currently done in the Laboratory of CSIC-Madrid. The seminar of the current investigations at Laboratory of ACP-Belgrade was given in CSIC on 11th July under the title "Binary Collisions of Electrons with Metal Atoms and Biomolecules".

Description of the main results obtained

Calculations of the electron scattering by glycine and alanine were carried out and the results for a wide range of electron impact energies (1-10,000 eV) had been obtained. Both differential and integral cross sections were calculated in IAM approximation.

Proper effective path length correction factor was found for the present targets and experimental geometry. Relative differential cross sections were obtained from raw experimental data of angular distributions at four impact energies (20, 40, 60 and 80 eV).

By normalization and extrapolation of experimental data points, absolute DCS values for elastic electron scattering by glycine and alanine were obtained. These data are finally compared with present calculations and very good agreement was achieved.

In assembling the new apparatus for measuring the partial ionization cross sections, the stage of finalizing the electron gun, Faraday cup, interaction volume and detection of electrons and ions was reached. This is done in conditions of high vacuum obtained by two turbo pumps.

Future collaboration with host institution

Future collaboration will include the publishing the jointly obtained results on electron elastic scattering by glycine and alanine molecules. These data are needed in order to complete the picture of electron interaction with single molecules as well as to investigate the role of low and medium energy electron in radiation damage to living cells.

Collaboration of other molecular targets was considered and planned. Also, the collaboration on atomic targets such as Zn atom was initiated. The intrinsic problem of IAM approximation used in the present calculations was recognized and will be one of the objectives of the further collaborations.

Compatibility of present experimental set-ups in two laboratories, Laboratory of CSIC-Madrid and Laboratory of ACP-Belgrade is recognized and will be used in further planning in the activities of electron scattering experiments. Also, combing the calculations with experimental investigation of the same collision processes will lead to overcoming the present limitations of both used methods.

Projected publications/articles resulting or to result from grant

The first result to come is the presentation the current work at the next EIPAM meeting in Malta, from 16th to 20th September. There, the results for electron elastic scattering will be presented with the pointing out of the limitations of the experiment and theory and their complementarity.

The full publication of the results is expected in pear review scientific journal. The elastic electron cross sections by glycine and alanine molecules have been in preparation for publication.

Other comments

The visit was very stimulating for the exchange of ideas and also joint work on the selected targets. Three main components of the scientific work were covered during the visit: processing of raw experimental data obtained earlier, calculations of the same processes and starting with development of the new experimental set-ups.

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HOST STATEMENT FORM

21st July 2006

I am pleased to state that the visit of Dr. Bratislav Marinkovic was underdone with success and according the planed activities. The joint work was done as explained in the Scientific Report presented by grantee, Dr. Marinkovic. We have also organized a seminar in the CSIC Department for Atomic, Molecular and Aggregate Physics and the letter of certification is also enclosed into this document. We are sure that this visit will contribute significantly to our future collaboration and increase the number of joint publications.

Dr. Gustavo Garcia

Instituto de Matemáticas y Física Fundamental (IMAFF)
Consejo superior de investigaciones Científicas (CSIC)

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Madrid, 11 de Julio de 2006

Prof. Bratislav Marinkovic
Center for Atomic and Subatomic Physics, Belgrade Institute of Physics,
Pregrevica 118, 11080 Belgrad-Zemun,
Serbia and Montenegro

With this letter we certify and express our gratitude for the scientific contribution of the **Prof. Bratislav Marinkovic** in the series of seminars of the Departamento de Física Atómica, Molecular y de Agregados of the CSIC. The seminar took place on July 11, 2006, and their title was:

"Binary collisions of electrons with metal atoms and biomolecules"

yours faithfully

INSTITUTO DE MATEMÁTICAS Y FÍSICA FUNDAMENTAL
CSIC

Prof. Gerardo Delgado Barrio
Director del INSTITUTO DE MATEMÁTICAS Y FISICA FUNDAMENTAL

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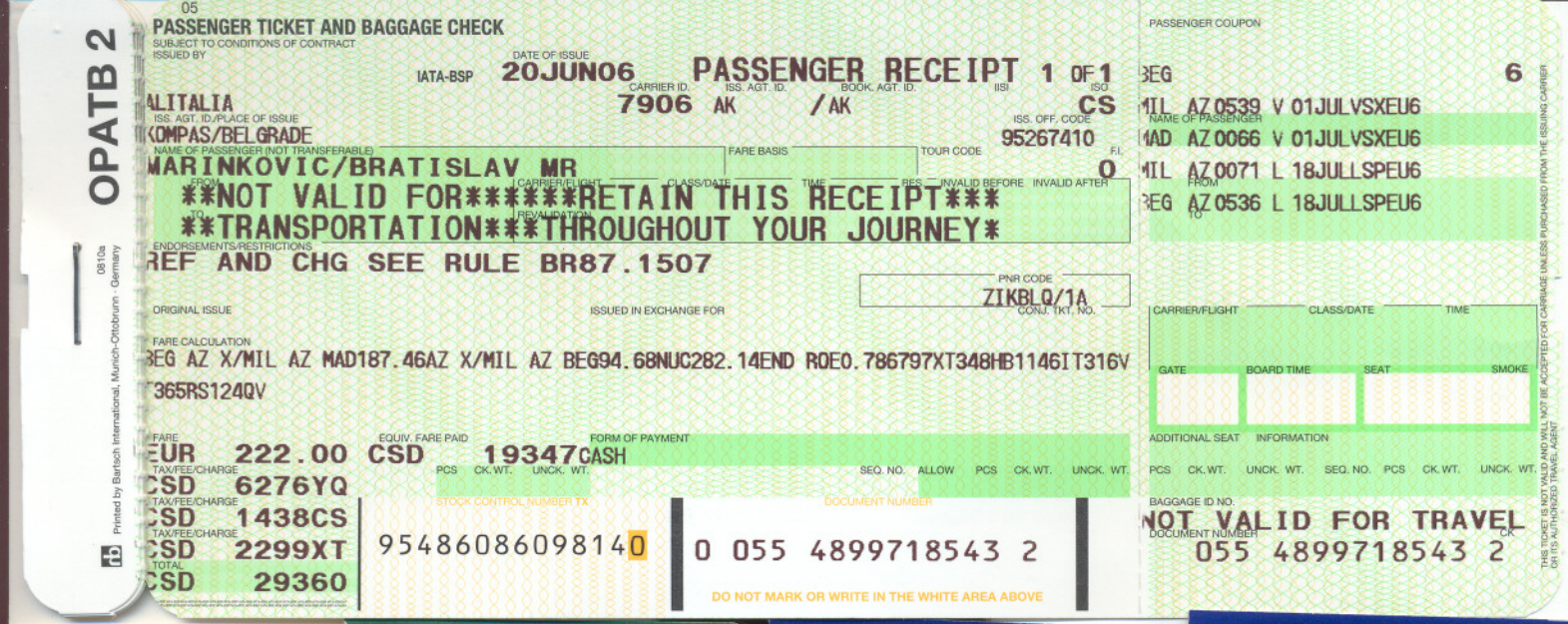

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FRA
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Gate A24
Boarding Time 1900
Seat 14F
NONSMOKER
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Boarding Time 2115
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Obilićev venac 26

Beograd 20 JUN 2006

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