

An Open Code Perturbative Model for Ionization Collisions

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National Atomic Energy Commission - ARGENTINA

24th Meeting of the A+M Data Centres Network (2017)

BARILOCHE ATOMIC CENTRE



- ✓ 1.7 MeV tandem accelerator
- ✓ 300 keV and 100 keV accelerators
- ✓ TOF-ISS and XPS, UPS, AES, SIMS spectroscopy
- ✓ STM and AFM microscopes
- ✓ COLTRIMS

1.7 MEV TANDEM ACCELERATOR



- ✓ Particle Induced X-ray Emission (PIXE).
- ✓ Rutherford Backscattering Spectrometry (RBS).
- ✓ Elastic Recoil Detection Analysis (ERDA).
- ✓ Nuclear Reaction Analysis (NRA).
- ✓ Wavelength Dispersive X-Ray Spectroscopy (WDS)

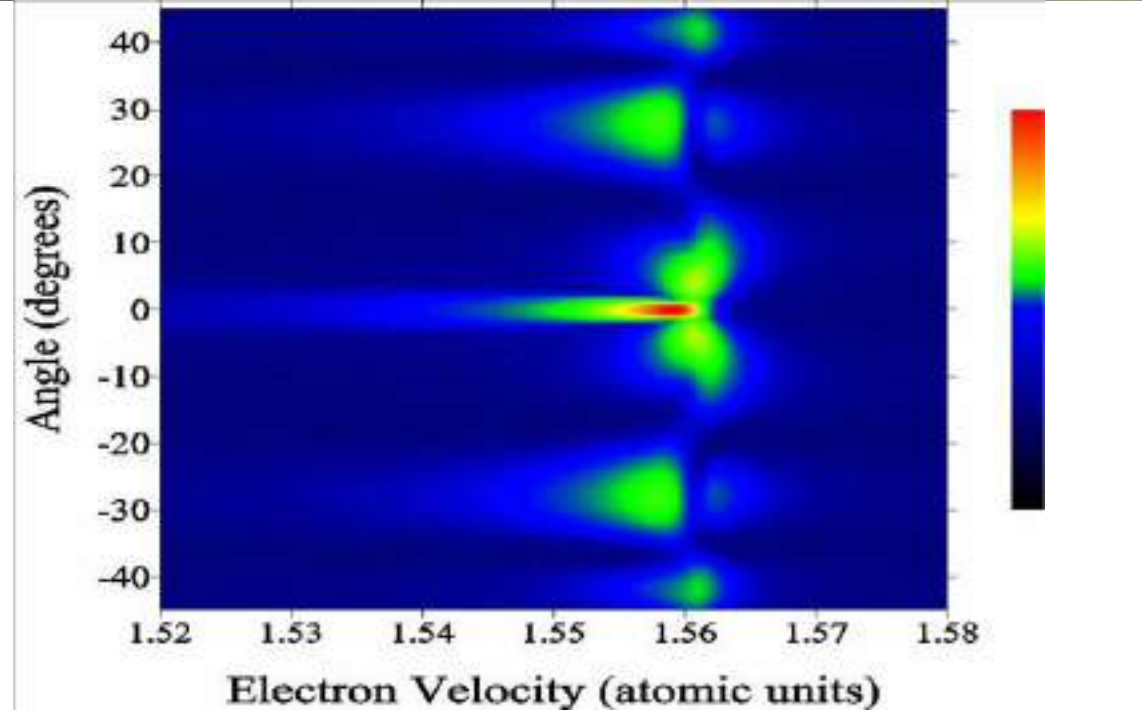
24th Meeting of the A+M Data Centres Network (2017)

BARILOCHE ATOMIC CENTRE



- ✓ CDW and C3 codes
- ✓ Classical Trajectory Monte Carlo (CTMC)
- ✓ Generalized Sturmian Functions
- ✓ Time-Dependent Close-Coupling
- ✓ MCNP, ...

THEORETICAL TECHNIQUES



- ✓ Projectiles: ion (nude and neutral), electrons, positrons
- ✓ Targets: Atoms, Simple and Complex (biological) Molecules, Surfaces, ...
- ✓ Channels: single and multiple ionization, charge exchange, transfer ionization, ...

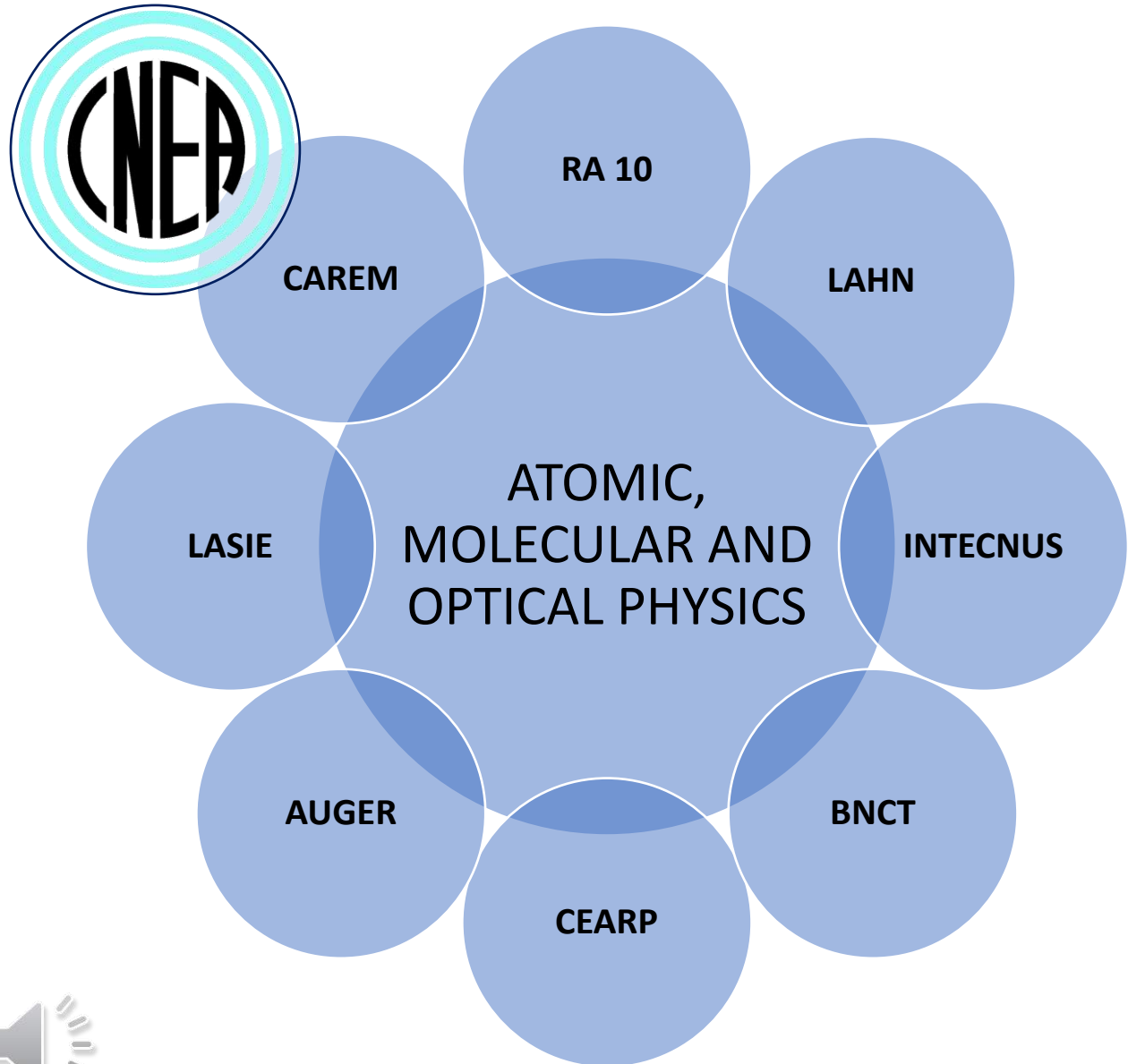
25th Meeting of the A+M Data Centres Network (2019)



It would not be a **good practice** to do AMO physics outside the context, priorities and needs of the Atomic Energy Commission.



25th Meeting of the A+M Data Centres Network (2019)



- ✓ RA 10: NUCLEAR RESEARCH REACTOR
- ✓ LAHN: NEUTRON BEAM LABORATORY
- ✓ INTECNUS: NUCLEAR MEDICINE
- ✓ BNCT: BORON NEUTRON CAPTURE THERAPY
- ✓ CEARP: PROTON THERAPY CENTRE
- ✓ AUGER: PIERRE AUGER LABORATORY
- ✓ LASIE: LASER SEPARATION ENRICHMENT
- ✓ CAREM: SMALL MODULAR REACTOR
- ✓ ...



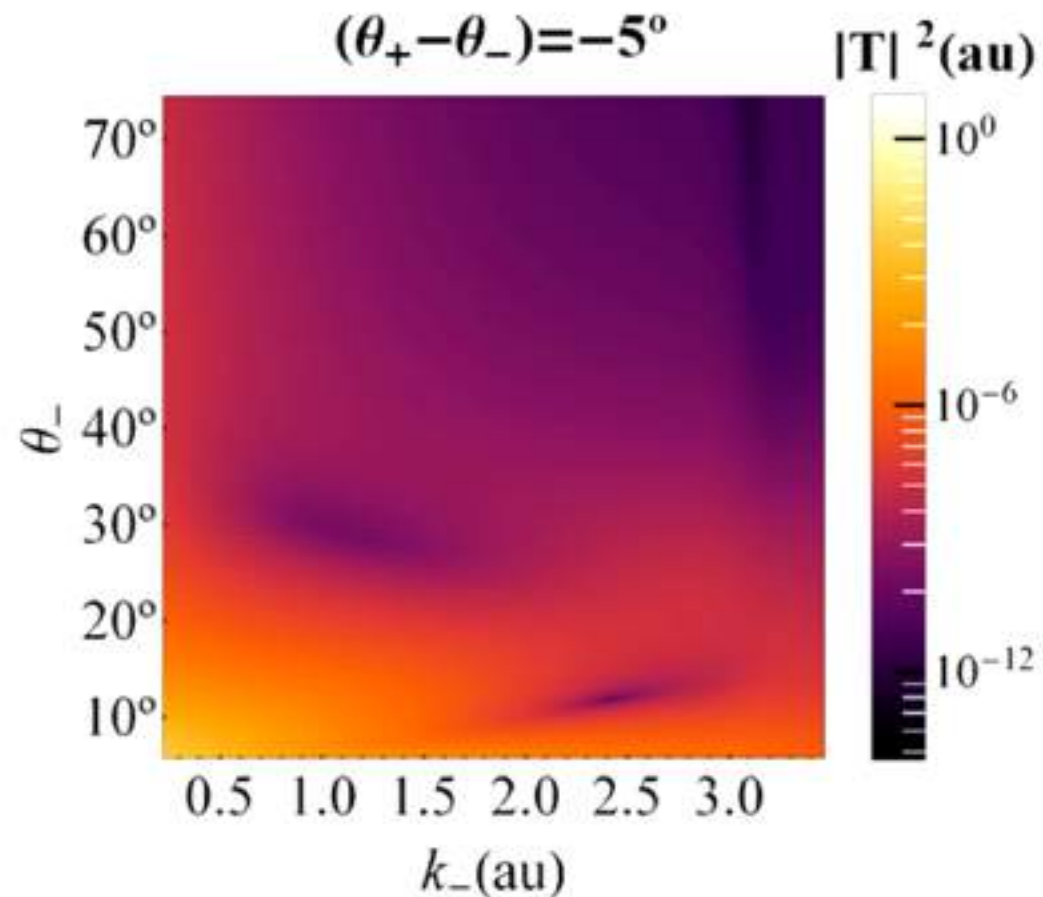
DATOS Y CÓDIGOS INFORMÁTICOS

NUCLEARES, ATÓMICOS, MOLECULARES Y ÓPTICOS



26th Meeting of the A+M Data Centres Network (2021)

An Open Code Perturbative Model for Ionization Collisions





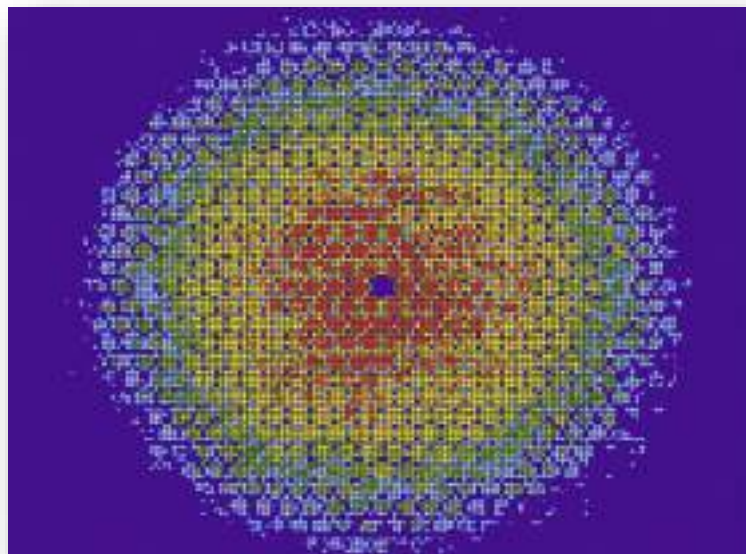
NEA

NUCLEAR ENERGY AGENCY

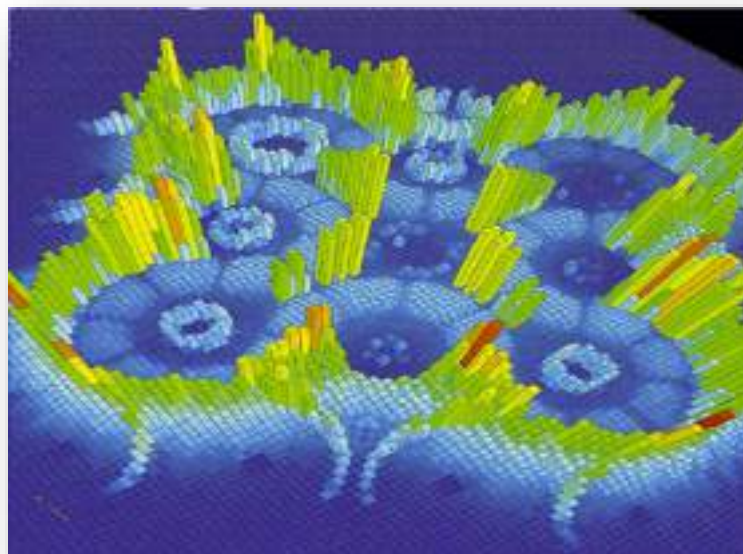
DATA BANK



The OECD/NEA's headquarters in Paris



COMPUTER PROGRAM
SERVICES (CPS)



NUCLEAR DATA
SERVICES (NDS)



THERMOCHEMICAL
DATABASE (TDB)





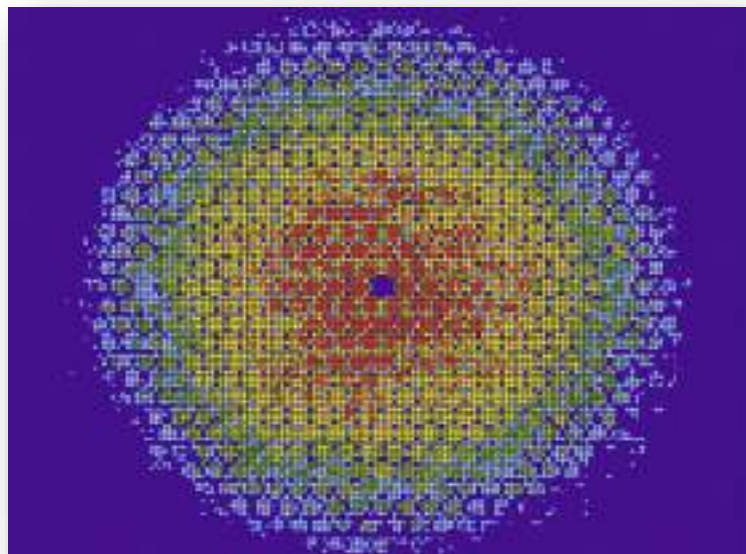
NEA

NUCLEAR ENERGY AGENCY

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COMPUTER PROGRAM
SERVICES (CPS)

MISSION

- to collect, test and distribute computer programs
- to organize training courses on the most popular computer programs
- to preserve and distribute integral experiment data, databases, processed libraries, benchmark and NEA safety joint projects.





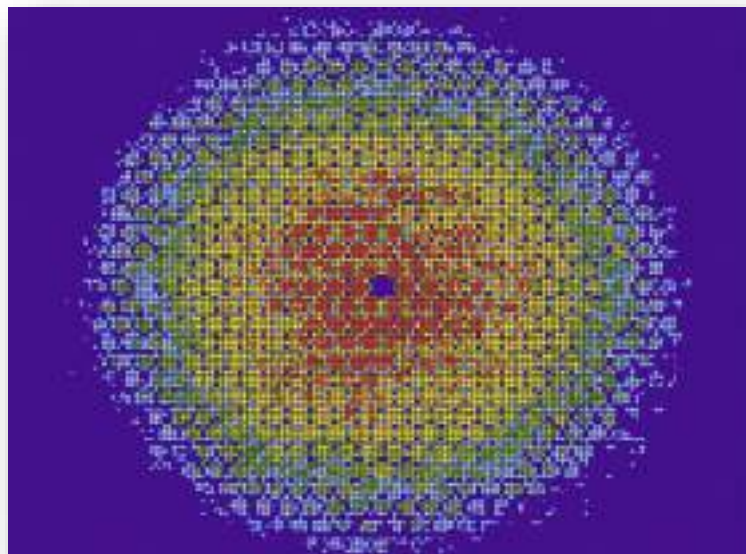
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COMPUTER PROGRAM
SERVICES (CPS)

OPEN SOURCE

- Free distribution (when possible) with individual licenses
- Streamlined online dispatch
- Collaborative (developers and end-users): GITLAB
- Training courses
- Statistics and Feedback

Task Force on the evolution of the Computer Program Services





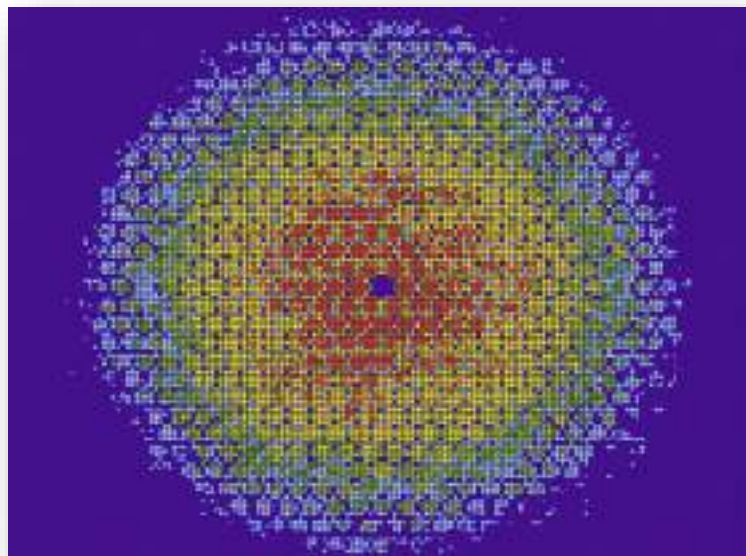
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COMPUTER PROGRAM
SERVICES (CPS)

GUESS

- How many Atomic, Molecular and Optical Physics Computer Programs are in the NEA catalogue?
- How many times are they requested per year?



List of Codes

Codes available through ONCORE

Name	Brief description	How to obtain the software
VSOP99/11	HTR pebble-type design and safety analysis	Available at: Registered users of ONCORE
STACY	V/HTR safety analyses for the quantification of fission product release from the fuel.	Available at: Registered users of ONCORE

Other codes



Online Computing

Below are some links to online computing resources for calculating plasma properties.

HEAVY: Cross sections for excitation and charge transfer for collisions between hydrogenic targets and bare ions.

AAEXCITE: An interface to average approximation cross sections for calculating electron impact cross sections for atomic ions.

RATES: Results from collisional radiative calculations of plasmas carried out with the Los Alamos modeling codes are available. Interpolations allow the user to obtain total radiated power, average ion charge, and relative ionization populations in a steady state plasma.

FLYCHK: An interface to the FLYCHK code available at NIST, which generates atomic level populations and charge state distributions for low-Z to mid-Z elements under NLTE(Non-Local Thermodynamic Equilibrium) conditions.

FAC (Flexible Atomic Code): A complete set of collisional and radiative data of atoms from Z=2 (Helium) to Z=14(Silicon).



Online Computing

Below are some links to online computing resources for calculating plasma properties.

[HEAVY](#): Cross sections for excitation and charge transfer for collisions between hydrogenic targets and bare ions.

This is your gateway to the calculation of cross sections for excitation, ionization and charge transfer in heavy particle collisions, using codes developed by A. Dubois, J.P. Hansen and P. Fainstein. [Click here](#) for a description of the method and references for the excitation and charge exchange code of Dubois and Hansen. [Click here](#) for a description of the method and references for the ionization code of Fainstein.

Use of the interface to run the code is restricted to registered users. If you wish to run the code, please contact us with your request, including your name, institution and brief reason for wishing to run the code.

[Click here](#) to submit your request.



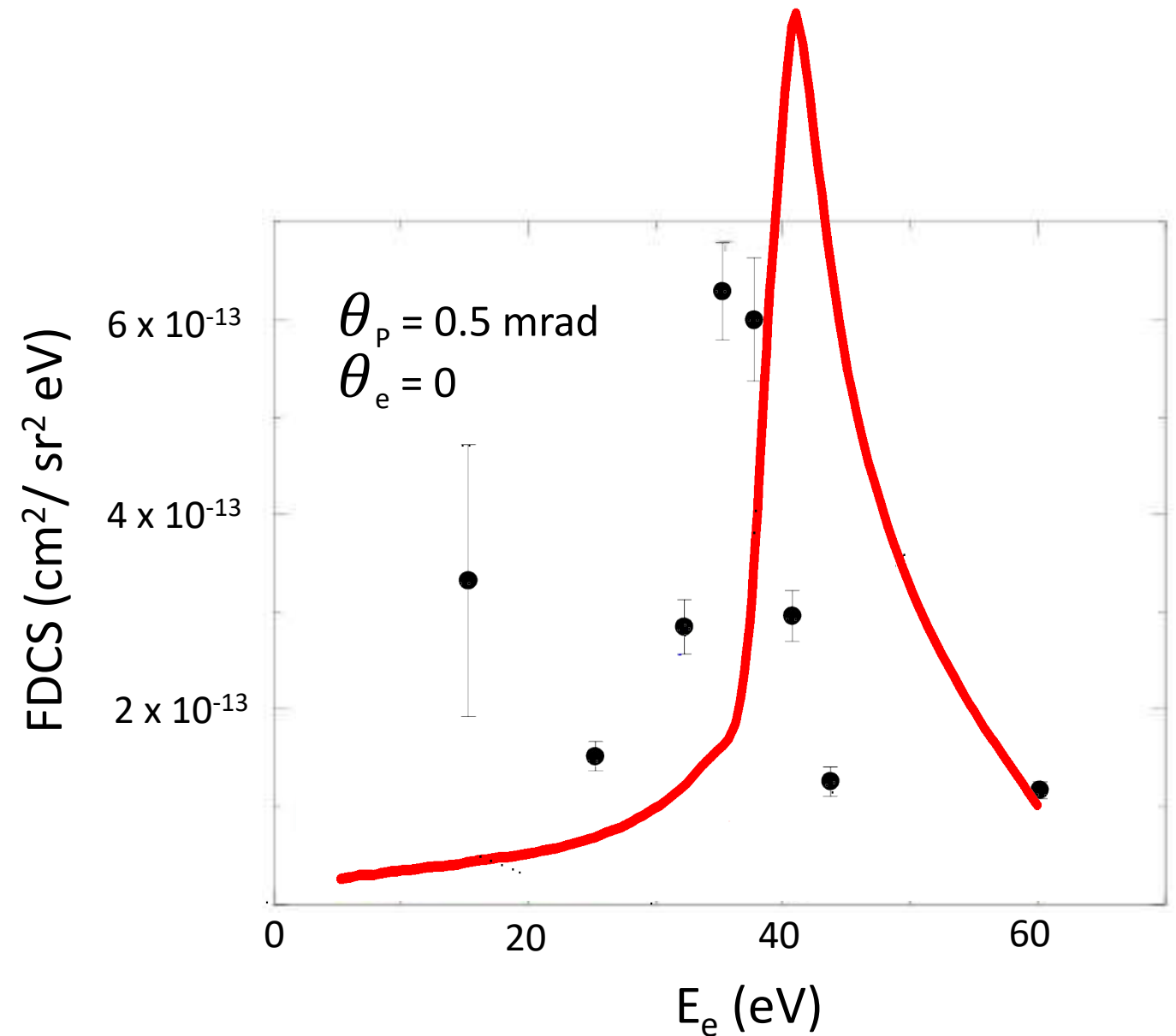


	Single Ionization	Single and multiple ionization
Process		
Developers	P Fainstein, V Ponce, R Rivarola	
Model	CDW EIS Continuum Distorted Wave Eikonal Initial State	
Target	Hydrogenic (1s, 2s, 2p)	Atoms and molecules
Electron – electron interaction	Independent electron model	
Projectile-target relative motion	Classical (straight-line, constant velocity v) a.k.a. Impact parameter approximation	
Projectile	Bare ion (Z)	
Velocity v (atomic units)	$v > Z$	
Open code	No	

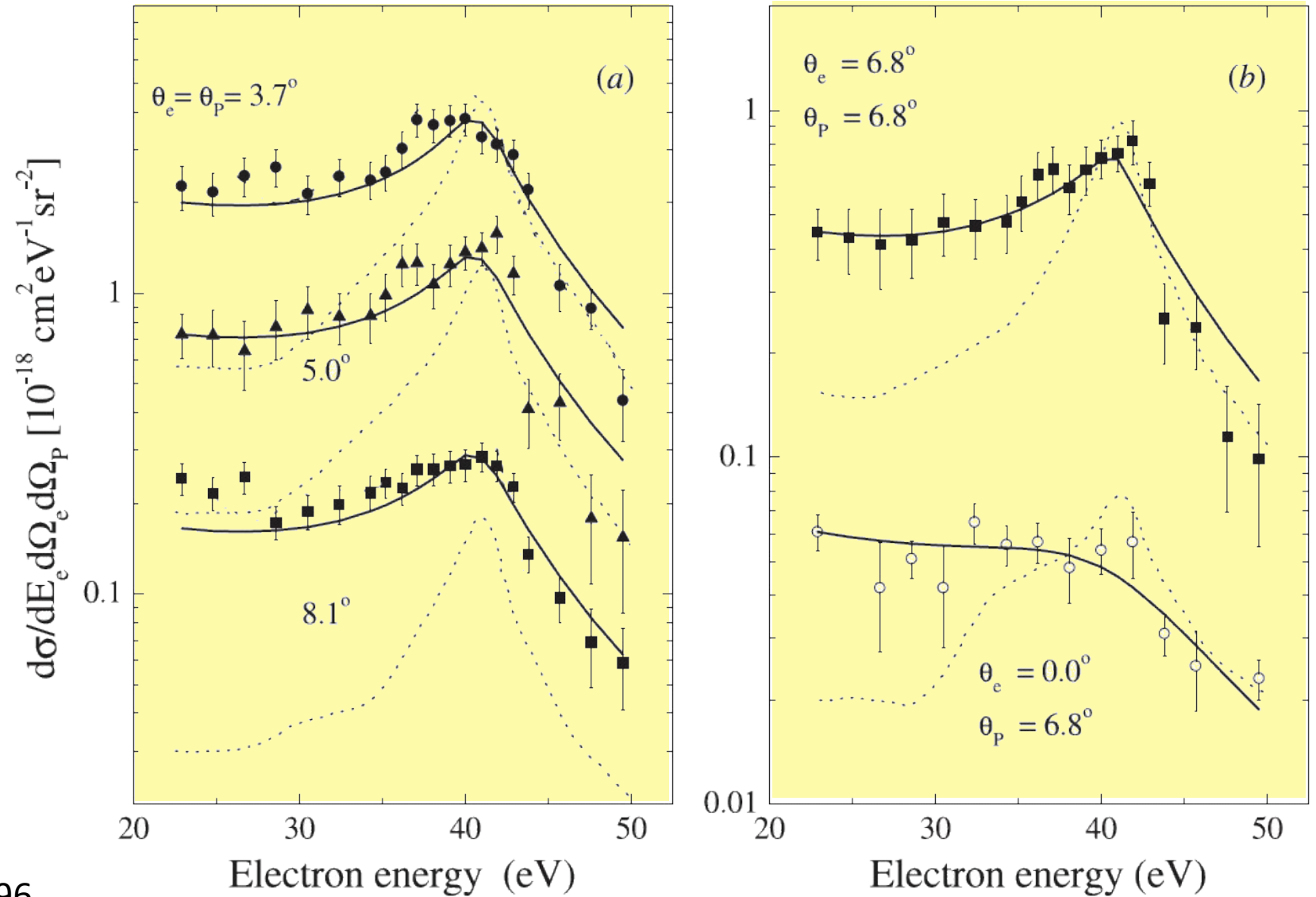
Process	Single Ionization	Single and multiple ionization
Developers	P Fainstein, V Ponce, R Rivarola	F Navarrete, J Fiol, Barrachina
Model	CDW EIS Continuum Distorted Wave Eikonal Initial State	C3 Correlated three-body Quantum Distorted Wave
Target	Hydrogenic (1s, 2s, 2p)	Atoms and molecules
Electron – electron interaction	Independent electron model	
Projectile-target relative motion	Classical (straight-line, constant velocity v) a.k.a. Impact parameter approximation	Quantum mechanical All interactions are considered on an equal footing.
Projectile	Bare ion (Z)	Ion, positron, electron, ...
Velocity v (atomic units)	$v > Z$	$v \geq 1$
Open code	No	Yes



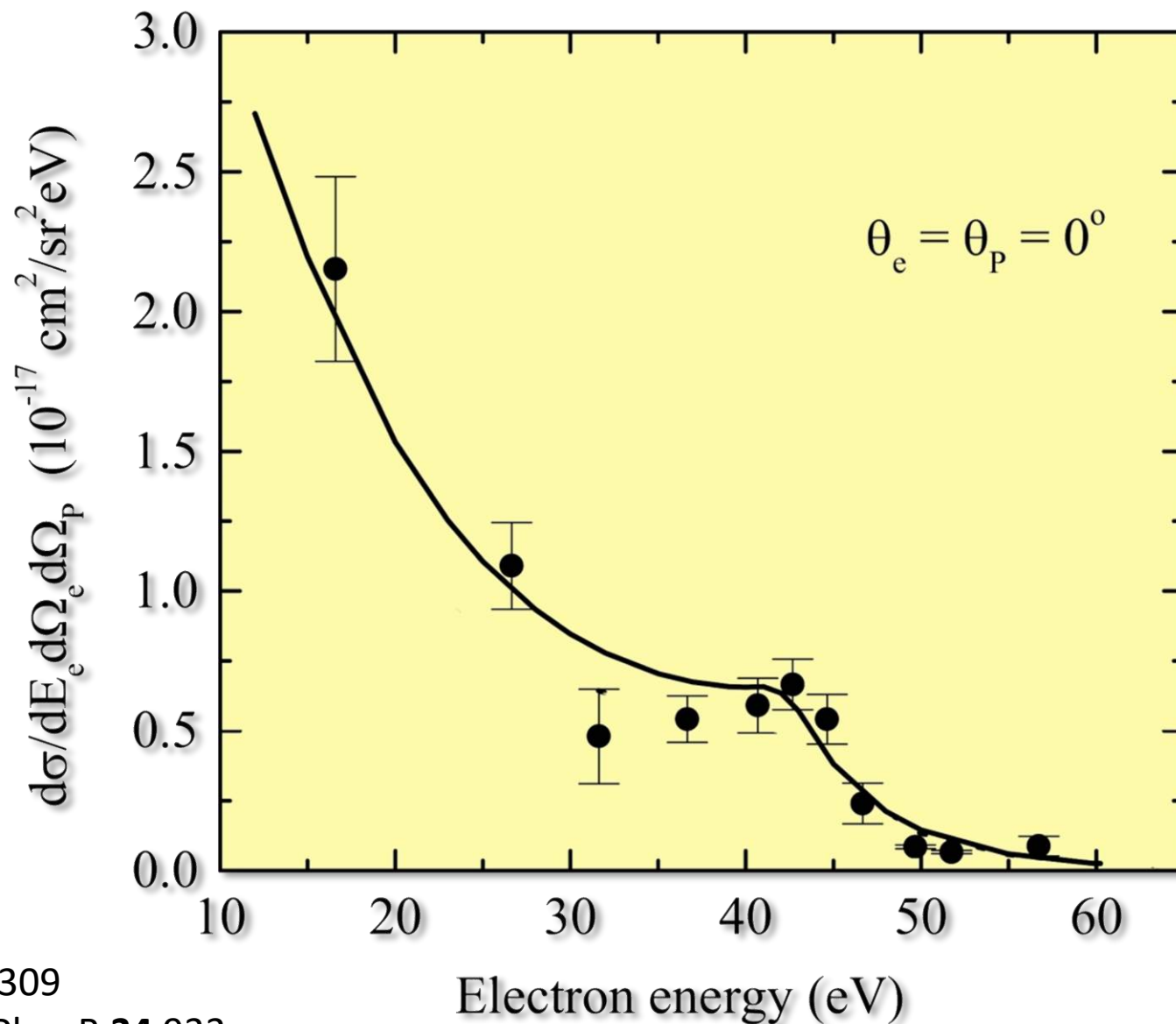
Ionization of He by the impact of 75 keV protons



Ionization of Ar by the impact of 75 keV protons



Ionization of H₂ by the impact of 100 eV positrons



Kövér A and Laricchia G 1998 Phys Rev Lett **80** 5309

Figi J, Rodriguez V D and Barrachina R O 2001 J Phys B **34** 933

A brief history of C3 and CDW-EIS in our LAB

SOVIET PHYSICS JETP

VOLUME 18, NUMBER 5

MAY, 1964

*ON A CERTAIN MODEL FOR CALCULATION OF THE EFFECTIVE CROSS SECTIONS FOR
EXCITATION OF ATOMS*

L. VAĪNSHTEĪN, L. PRESNYAKOV, and I. SOBEL'MAN

P. N. Lebedev Physics Institute, Academy of Sciences, U.S.S.R.

J. Exptl. Theoret. Phys. (U.S.S.R.) 45, 2015-2021 (December, 1963)

1963

PHYSICAL REVIEW A

VOLUME 21, NUMBER 2

FEBRUARY 1980

Ionization and electron capture to the continuum in the H^+ -hydrogen-atom collision

C. R. Garibotti* and J. E. Miraglia*

Centro Atómico Bariloche[†]-Instituto Balseiro,[‡] 8400 S. C. de Bariloche, R. N., Argentina

(Received 12 February 1979)

1980



C3

J. Phys. B: At. Mol. Opt. Phys. **24** (1991) 3091-3119. Printed in the UK

Two-centre effects in ionization by ion impact

Pablo D Fainsteint, Victor H Poncet† and Roberto D Rivarola‡

† Centro Atómico Bariloche and Instituto Balseiro, 8400 Bariloche, Argentina

‡ Instituto de Física Rosario (Consejo Nacional de Investigaciones Científicas y Técnicas and Universidad Nacional de Rosario), Avenida Pellegrini 250, 2000 Rosario, Argentina

1991



CDW EIS

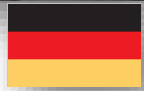


An Open Code C3 Model for Ionization Collisions

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Francisco Navarrete



Juan Fiol



Raúl Barrachina



THANK YOU FOR
YOUR ATTENTION

National Atomic Energy Commission (Argentina)



University of Rostock (Germany)

