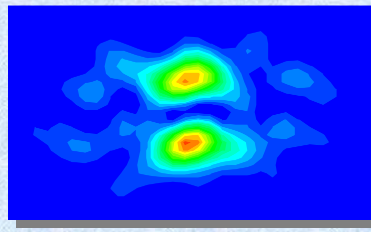
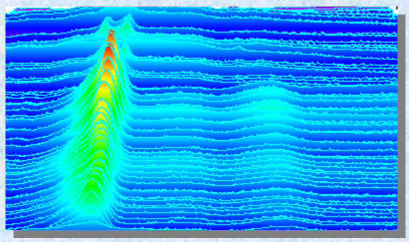
The ORNL Controlled Fusion Atomic Data Center

ATOMIC DATA FOR FUSION





Overview

Experimental work

Theoretical work

The ORNL Atomic Physics Group

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* departed in last 2 years

Data Center Staff

^ Data Center Consultants

The ORNL Atomic Physics Group

The Multicharged Ion Research Facility (MIRF)

SciDAC Scientific Discovery through Advanced Computing

Theoretical Atomic Physics

The Controlled Fusion Atomic Data Center (CFADC)

ATOMIC DATA FOR FUSION

The Controlled Fusion Atomic Data Center

- Established in 1958 by Clarence Barnett, early partnership with U.S. National Bureau of Standards (now NIST), persistent division of responsibility – CFADC: collision and PSI data, NIST: spectroscopic data
- International coordination through the IAEA Data Center Network, participation in the ALADDIN network, IAEA CRPs
- Makes available a range of collected & evaluated data and collisional-radiative modeling software – e.g. Redbooks, ADAS, MIRF data
- Answers direct requests from the fusion and broad plasma science communities for data collection, production - targeted, focused data production

CFADC Bibliography

- Among the chief activities of the data center since its inception has been to provide a published, categorized bibliography of atomic data references of interest to fusion
- It answers direct needs of fusion for data and serves a basis for data evaluation & recommendation
- Since 1995 available through a web search engine, greatly leverage human resources, 1978-present approximately 1000 additional entries each year
- Published as major portion of the IAEA *International Bulletin on Atomic and Molecular Data for Fusion*
- A new storage and retrieval system based on Microsoft's **Access** was developed, new server installation and continued software development

CFADC Data Resources – change in approach

- Traditional data center approach (1958 – c. 1995)

  Very broad projects of data collection, evaluation, and recommendation (e.g. Redbooks) using a large group of technical & clerical staff and consultants

- New data center approach (c. 1995 – present)

  Targeted, focused data production (e.g. from community requests, IAEA Coordinated Research Programs, SciDAC projects)

  + on-line bibliography, ADAS, ALADDIN, and answering of 'small' data requests

CFADC 'small' data requests

- The CFADC receives about two dozen 'small' data requests per year, examples from the past few months include
  - Hydrogen beam heating, need for sublevel specific excitation cross sections, access to ADAS
  - Measure continuum coming from plasmas, need high energy electron scattering from hydrogen
  - Modeling damage to walls via neutrals from charge transfer, need proton-impurity, and impurity-impurity charge transfer cross sections

CFADC 'large' data requests

- The CFADC answers much larger requests for data through a variety of channels, leading to major projects
  - direct requests from the fusion community, e.g. multi-year project on elastic and related transport cross sections, DEGAS-2; other transport experiments at DIII-D (carbon) and Alcator C-Mod (Ar)
  - IAEA Coordinated Research Programs, e.g. vibrationally resolved molecular hydrogen collision data, IAEA CRP "Atomic and Molecular Data for Fusion Diagnostics," 2001-04
  - workshops, e.g. on PSI, MAR, generating a wide range of identified needs for data from plasma science participants

Participation in recent IAEA Coordinated Research Programs

- Charge exchange cross section data for fusion plasma studies, 2000
- Atomic and plasma-wall interaction data for fusion divertor modeling, 2000
- Atomic and molecular data for fusion diagnostics, 2004
- Atomic and molecular data for plasma modeling (hydrocarbon data), 2007
- Data for surface composition dynamics relevant to erosion processes, 2007

Recent Workshops and Conferences

"Atomic and Molecular Processes in Divertor Plasma Volume Recombination" – CFADC Workshop 2000

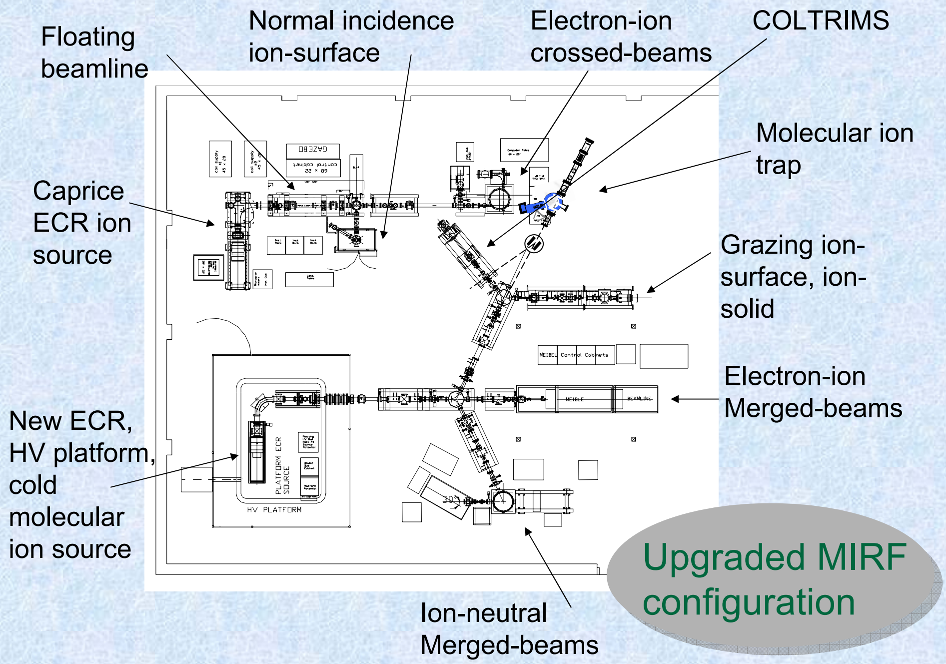
"International Conference on Photonic, Electronic, and Atomic Collisions" – ICPEAC, 2001

"13th APS Topical Conference on Atomic Processes in Plasmas" – APiP, 2002

"3rd International Conference on Atomic and Molecular Data and Their Applications" – ICAMDATA, 2002

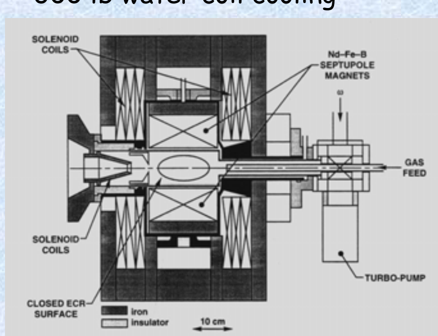
"New Directions in Particle-Surface Interactions for Fusion" – CFADC Workshop 2005

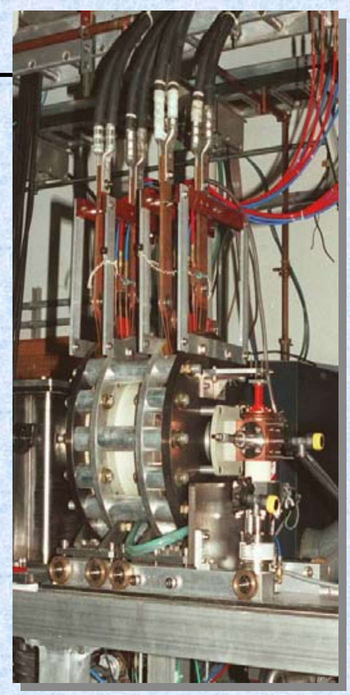
"37th APS Division of Atomic, Molecular, and Optical Physics Annual Meeting" – DAMOP, 2006



Caprice ECR Ion Source

- Produces a broad range of charge states and species
- Gas feed, mini-oven, biased sputter probe
- 50 kW coil power, RF, analyzer, pumps, controls
- 300 lb water coil cooling





All Permanent Magnet ECR Ion Source

- Performance better than Caprice source
- All permanent magnet design, no axial field power supplies (50 kW savings)
- No separate cooling loop for hexapole
- Optimum for placement on high voltage platform

Deceleration Optics for Floating Beamline

- Five element optic developed for floating ion-surface scattering experiment will be used on the new Caprice ECR floating beamline

MIRF upgrade: motivation

We are developing unique tools to address

- Volume molecular processes in the cool/dense edge and divertor plasmas
- Plasma-material interface, wall erosion, tritium retention

Reactions
Example: Molecular Assisted Recombination with hydrocarbons
$H^+ + C_xH_y \rightarrow H + C_xH_y^+$ (CX)
$e^- + C_xH_y^+ \rightarrow \Sigma\, C_{x-k}H_{y-l} + H$ (DR)
$H^+ + C_{x-k}H_{y-l} \rightarrow H + C_{x-k}H_{y-l}^+$
$e^- + C_{x-k}H_{y-l}^+ \rightarrow \Sigma\, C_{x-i}H_{y-j} + H$
… catalytic reaction continues

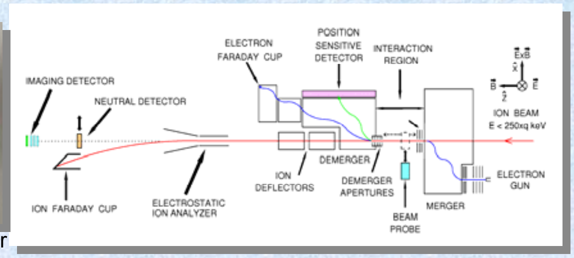
CH_4 / C_2H_6 / C_3H_8 are 10/30/40 times more efficient recombining H^+ from core plasma than H_2

Species
Fuel: H_2^+, H_3^+, plus D,T → H substitutions
Hydrocarbons: CH_x^+, $C_2H_y^+$ … $C_mH_n^+$
Impurity Hydrides: LiH_x^+, BeH_x^+, BH_x^+, OH_x^+…
Others: O_2^+, CO^+, CO_2^+, HCO^+ …
Surface: various carbon containing materials, W, …

Merged electron-ion beams apparatus

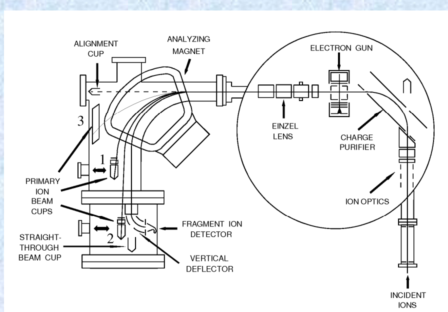
particle counting detector

fragment imaging detector



- ECR source on 250-kV platform enables detection of neutral fragments from DR
- Measurements of DR rate coefficients using particle counting detector
- Imaging of neutral fragments – study dynamics of dissociation
- Segmented SBD being developed will be energy- and position-sensitive down to 10 keV protons

Electron-ion collisions, crossed-beams

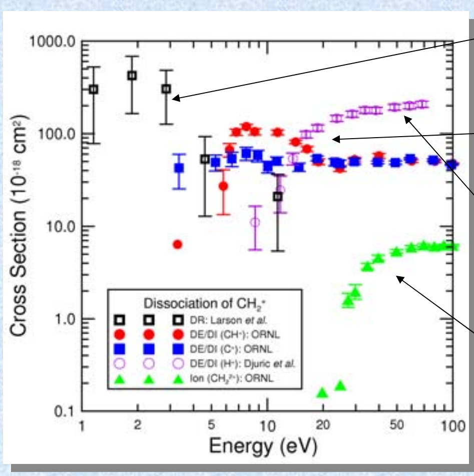


- Ions from ECR source interact at 90° with magnetically confined electron beam
- Product ions are magnetically analyzed and detected by CEM or fast discrete dynode detector
- Parent ions collected in one of 3 Faraday cups
- Electrons chopped to separate signal from background due to ionization on residual gas

Electron-driven hydrocarbon reactions

Process	σ (10^{-18} cm^2) 10 eV (DE only)		σ (10^{-18} cm^2) 50 eV (DE + DI)	
	Data in EIRENE Version 1, 2	MIRF exp.	Data in EIRENE Version 1, 2	MIRF exp.
$CH^+ \rightarrow C^+$	247	77	198	100
$CH_2^+ \rightarrow CH^+$	0, 23	105	101, 83	51
$CH_2^+ \rightarrow C^+$	0, 9	44	91, 35	53
$CH_3^+ \rightarrow CH^+$	0, 9	17	84, 65	53
$CH_3^+ \rightarrow C^+$	0	4	83, 34	27

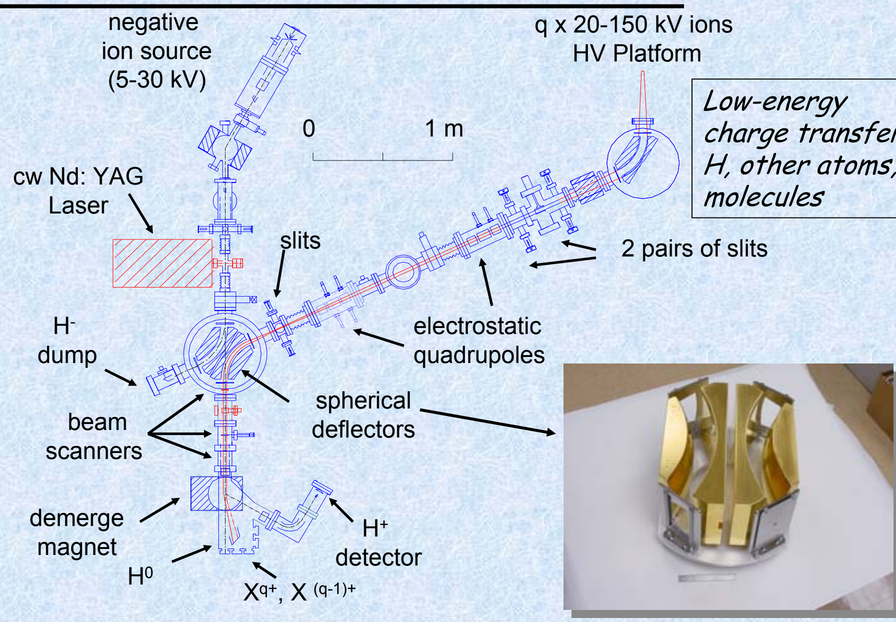
CH_2^+ Dissociation: "The Big Picture"



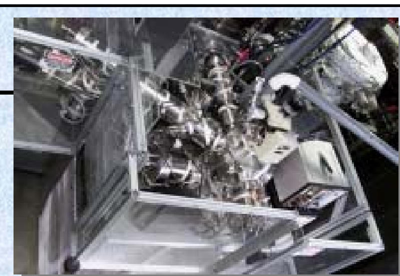
- In the 1-5 eV range, DR (black) is the dominant channel
- For E=5-15 eV, DE leading to CH^+ (red) and C^+ (blue) fragments is largest
- For E>20 eV, DE/DI producing H^+ (purple) fragments is dominant
- Surprisingly, ionization yielding CH_2^{2+} (green) ions is only a factor of 10 less than DE/DI of CH^+ and C^+ fragments at 100 eV

Upgrade: Ion-Atom Merged-Beams Apparatus

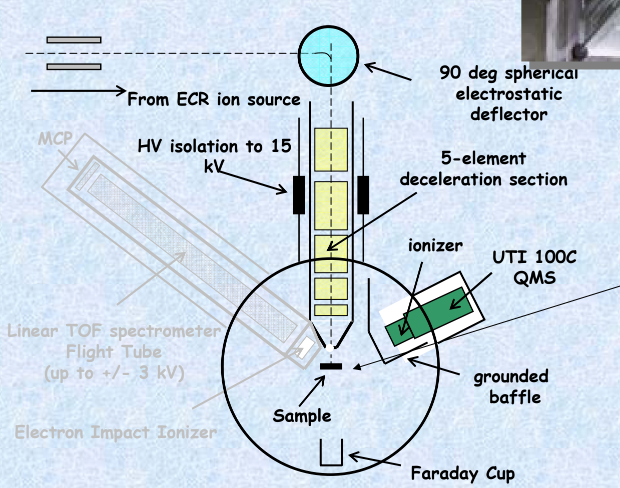
Low-energy charge transfer, H, other atoms, molecules



Particle-surface interaction apparatus



Recent focus on chemical sputtering, close collaboration with theory



e-beam sample heating up to T > 1200° C for annealing, reinitializing D sample inventory

David Schultz
Tatsuya Minami
ORNL

Mitch Pindzola
Francis Robicheaux
Eugene Oks
James Colgan
Stuart Loch
Auburn University

Don Griffin
Connor Ballance
Rollins College

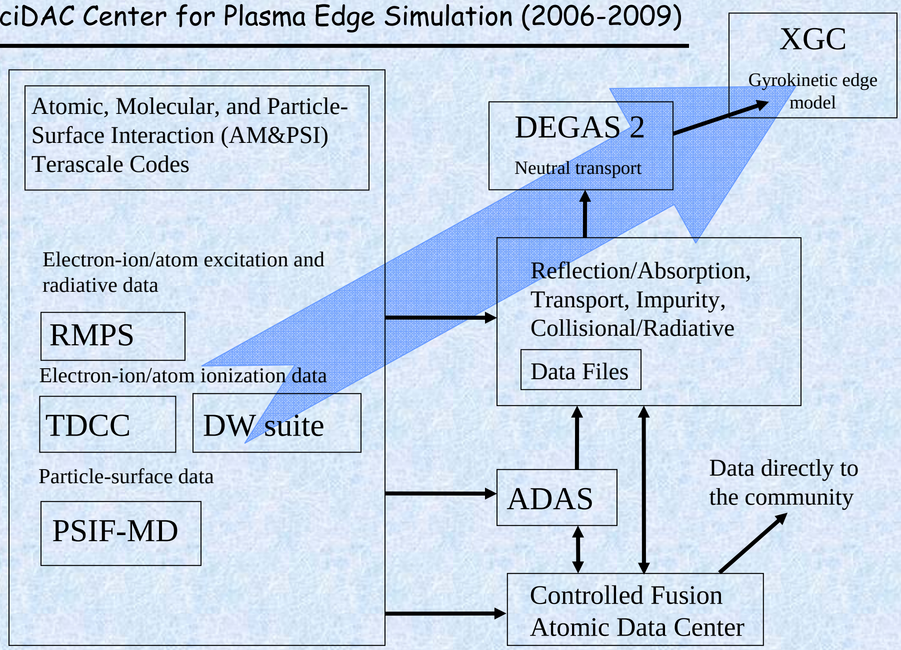
Computational atomic physics for plasma edge modeling (2001-2004)

Hugh Summers
Nigel Badnell
Strathclyde University
JET, UK

Phil Burke
Brendan McLaughlin
Queen's University, Belfast

Keith Berrington
Sheffield Hallam University

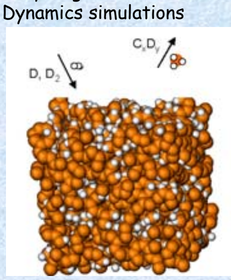
SciDAC Center for Plasma Edge Simulation (2006-2009)



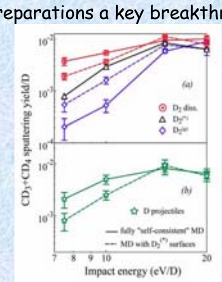
CPES AM&PSI progress in simulation of particle-wall interactions: D_2 + a:C

Science advances and data for neutral transport modeling – boundary interface

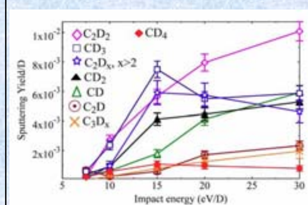
Very large scale Molecular Dynamics simulations

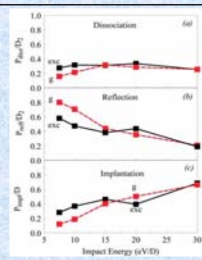


Self-consistent surface preparations a key breakthrough

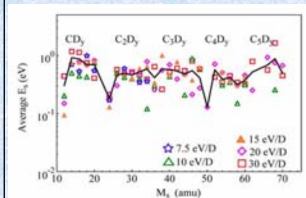


Hybridization structure and spectra of CD_x strongly correlated

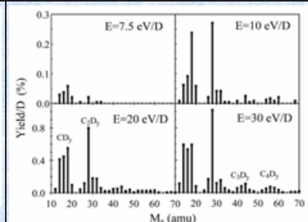




Data production for D_2 on deuterated amorphous carbon



Average translational kinetic energy of sputtered particles

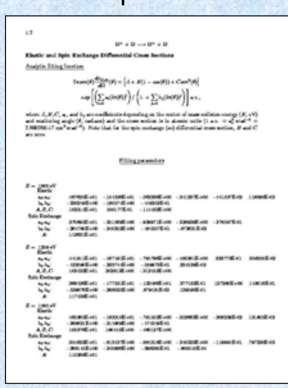


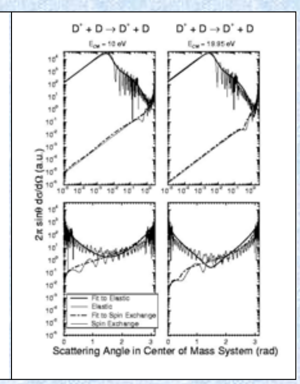
Sputtered particle spectra

Krstic and collaborators

Elastic scattering database

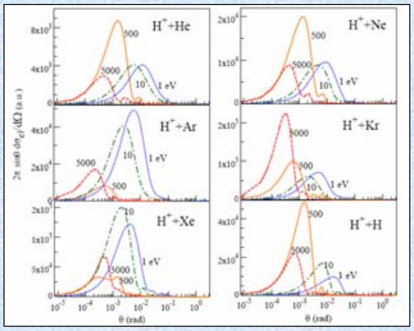
- All hydrogen isotopic variants if (H^+, H) + (H, H_2, He)
- Needed to model plasma charge, momentum, energy, and particle transport
- Fully quantal calculations of differential and integral elastic cross sections and transport moments
- Fitting formulae
- Scaling laws
- "Greenbook" Vol. 8
- Raw data on web
- 250 integral, 3000 differential cross sections

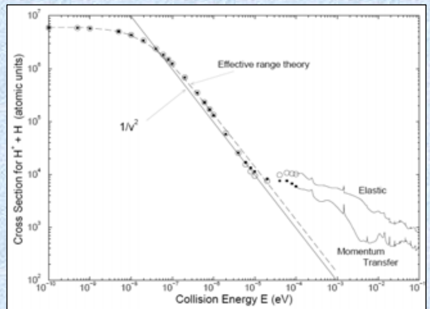


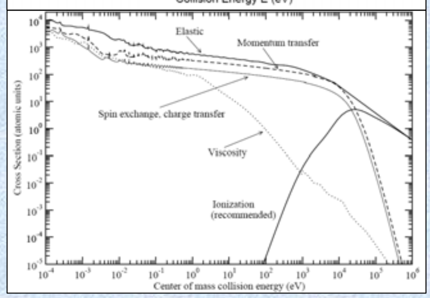


Elastic scattering database

- H^+ + H calculations extended to lower and to higher collision energies for astrophysical plasma applications
- H^+ + C, noble gases (He, Ne, Ar, Kr, Xe) for fusion applications
- H^+ + Li, Be, B, … calculations underway for fusion applications



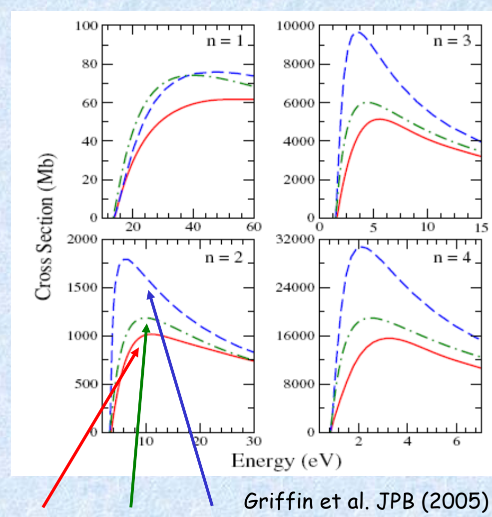




Data for scattering from excited states

e + H* ionization
n-bundled results

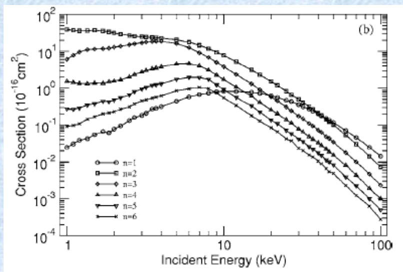
- Excited state populations in plasmas can significantly influence electron-impact ionization effective rates
- Standard models for this process have been shown to be inadequate by recent benchmark calculations

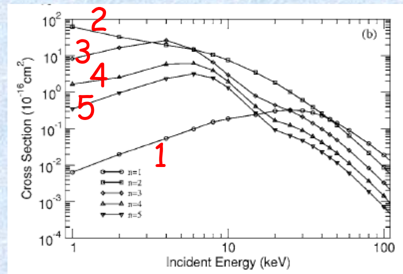


Griffin et al. JPB (2005)

Data for scattering from excited states

- Similar study for $H^+ + H(2s)$
  - Pilot database from extensive AOCC and CTMC calculations for excitation 2s → n,l and charge transfer 2s → n,l benchmarked by limited LTDSE-FD calculations

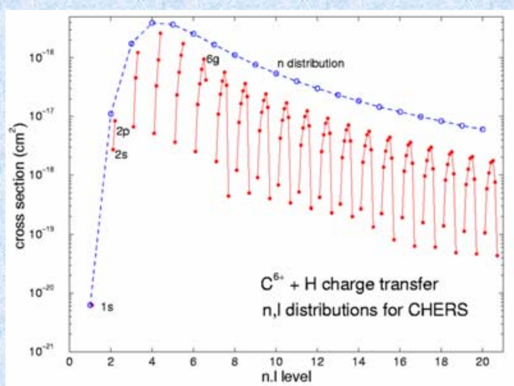




CTMC n-bundled charge transfer

AOCC n-bundled charge transfer

Inelastic data for impurities



- CTMC/AOCC/LTDSE/… calculations (excitation, charge transfer, ionization) can be made quickly enough and accurately enough to provide new data for a range of plasma science needs (DEGAS 2, SOLPS)

- Charge exchange recombination spectroscopy (CHERS), beam penetration (TRANSP, ONETWO)