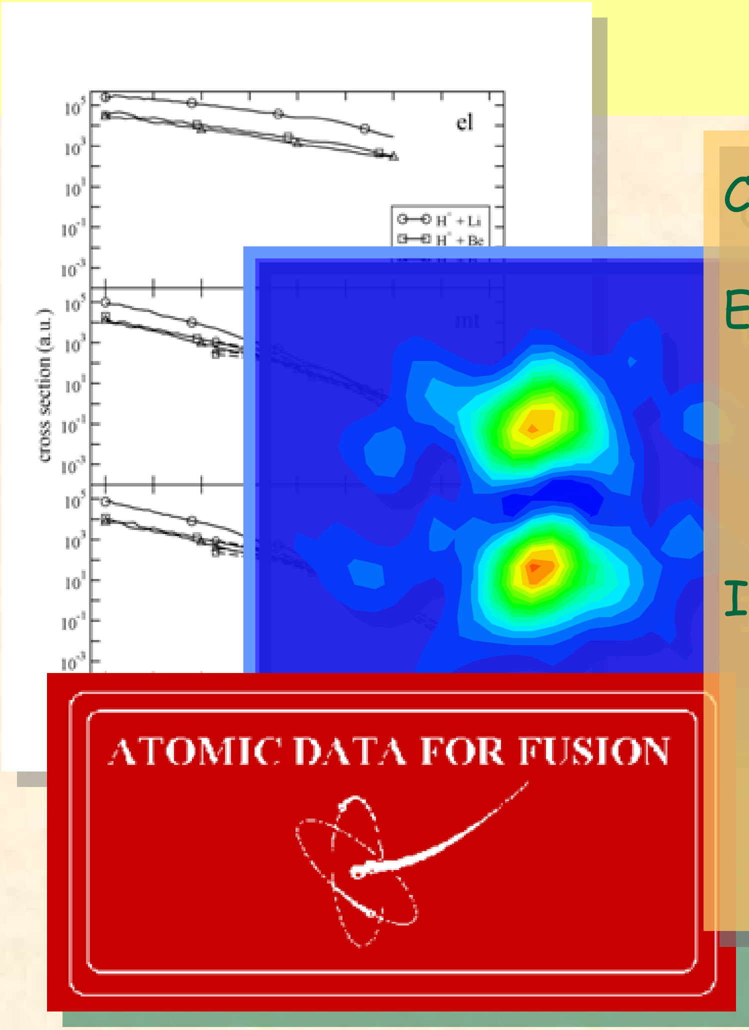
Recent calculations involving light species for fusion

David R. Schultz, Oak Ridge National Laboratory

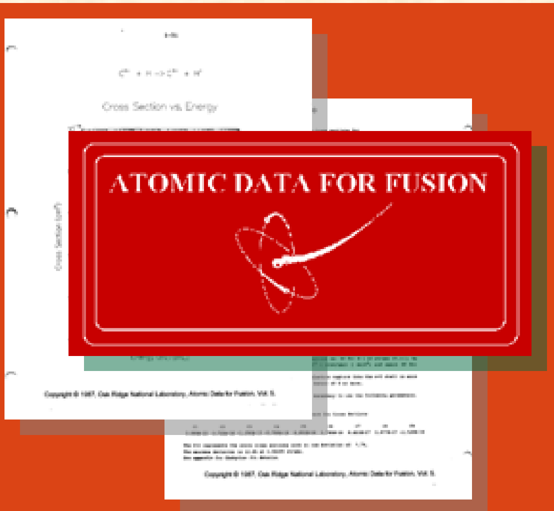


Context for the work

Elastic and transport processes
- Foundational database
- Recent light ion work
- Future calculations

Inelastic processes
- The LTDSE method
- Recent light ion work
- Beginning a fundamental calculation
- Future calculations

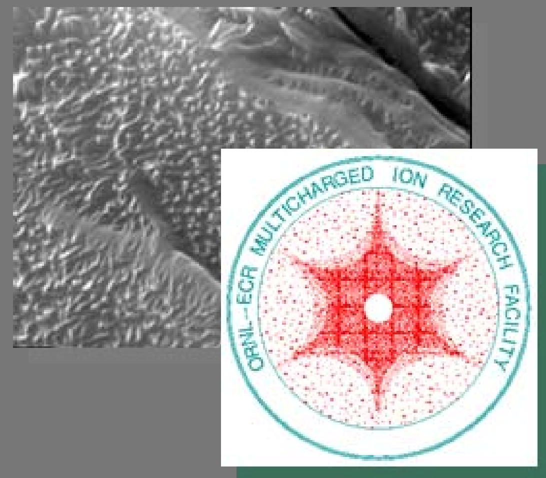
Context for the work



The Controlled Fusion Atomic Data Center

Collect, evaluate, and disseminate data to the plasma science community

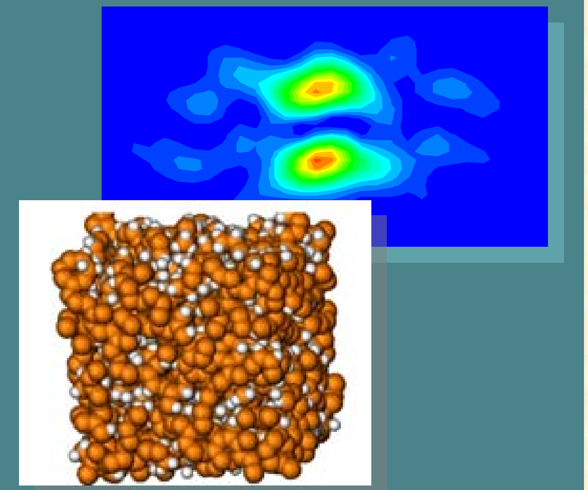
Schultz, Krstic, Ownby, Meyer, Havener, Bannister



The Multicharged Ion Research Facility

Study fundamental interactions among electrons, ions, atoms, molecules, and materials for plasma science

Meyer, Havener, Bannister, Hale, Vane, Deng, Harris, Draganic



Theoretical Atomic Physics

Develop and apply advanced computational methods in AM&PSI data production and basic science

Krstic, Schultz, Reinhold, Macek, Hui

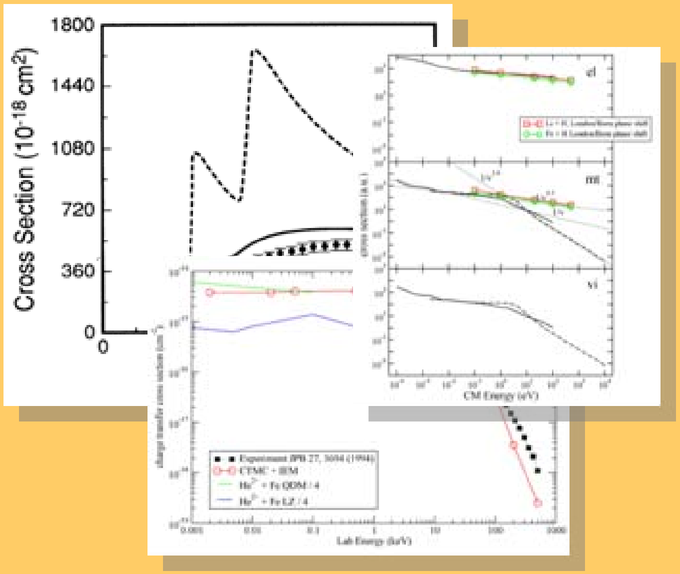
Answering Data Requests

Answering specific requests for data from the plasma science community is the highest priority

This is accomplished through

1. rapid feedback to requests using existing data sources or quick calculations, and
2. longer term data production projects

Recent example: Needed to provide a wide range of data (much of which did not exist) to a fusion laboratory evaluating transport of Fe in the scrape-off layer

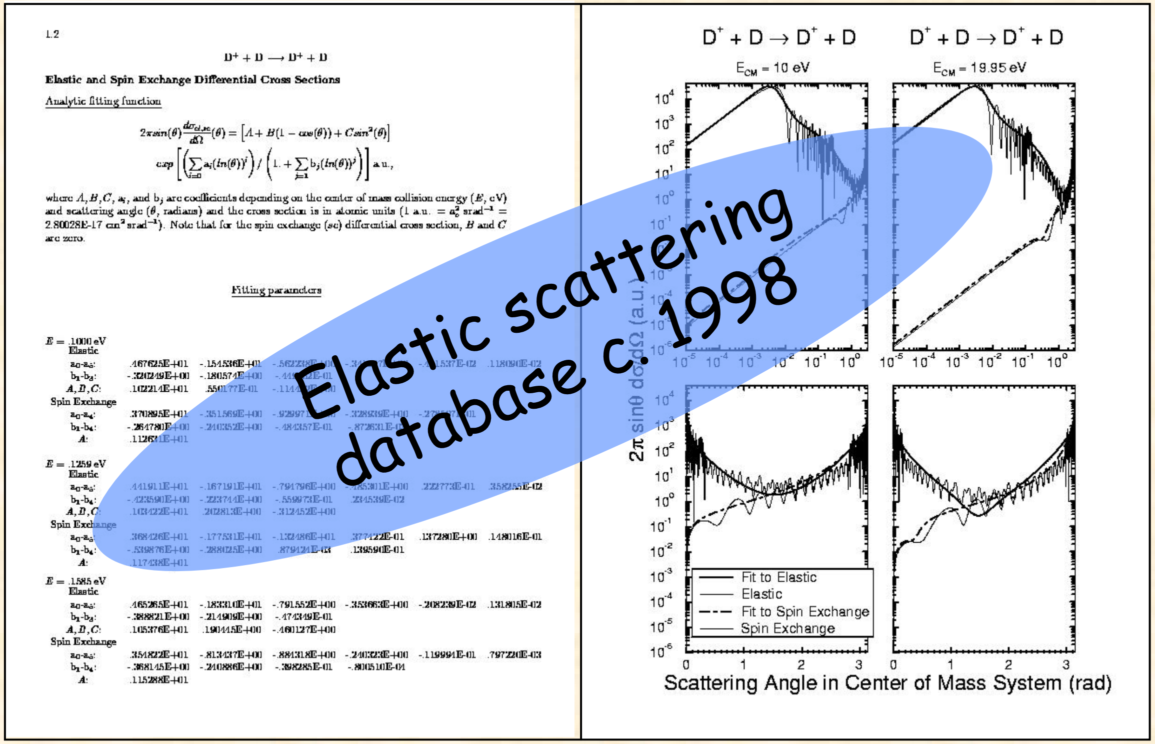


Fe + H, H_2 elastic scattering,
H^+ + Fe elastic scattering,
H^+ + Fe charge transfer,
e + Fe ionization

Some exiting data found, much estimated, longer-term project considered

Elastic and transport related data

- All hydrogen isotopic variants if (H^+, H) + (H, H_2, He)
- Needed to model plasma charge, momentum, energy, and particle transport – DEGAS 2 → Center for Plasma Edge Simulation
- Fully quantal calculations of differential and integral elastic cross sections and transport moments
- Fitting formulae
- Scaling laws
- IAEA “Greenbook” Vol. 8
- Raw data on web
- 250 integral, 3000 differential cross sections



1.2

$D^+ + D \longrightarrow D^+ + D$

Elastic and Spin Exchange Differential Cross Sections

Analytic fitting function

$$2\pi sin(\theta)\frac{d\sigma_{el,se}}{d\Omega}(\theta) = \left[A + B(1-cos(\theta)) + Csin^2(\theta)\right] exp\left[\left(\sum_{i=0} a_i(ln(\theta))^i\right) / \left(1 + \sum_{j=1} b_j(ln(\theta))^j\right)\right] \text{ a.u.},$$

where A, B, C, a_i, and b_j are coefficients depending on the center of mass collision energy (E, eV) and scattering angle (θ, radians) and the cross section is in atomic units (1 a.u. = a_0^2 srad^{-1} = 2.80028E-17 cm^2 srad^{-1}). Note that for the spin exchange (se) differential cross section, B and C are zero.

Fitting parameters

E = .1000 eV						
Elastic						
a_0-a_5:	.467625E+01	-.154536E+01	-.562238E+00	[illegible]	[illegible]	.118090E-02
b_1-b_3:	-.320249E+00	-.180574E+00	[illegible]			
A, B, C:	.102214E+01	.550177E-01	[illegible]			
Spin Exchange						
a_0-a_4:	.370895E+01	-.351569E+00	[illegible]	-.328939E+00	[illegible]	
b_1-b_4:	-.264780E+00	-.240352E+00	-.484357E-01	-.872631E-0[illegible]		
A:	[illegible]					
E = .1259 eV						
Elastic						
a_0-a_5:	.441911E+01	-.167191E+01	-.791796E+00	[illegible]	.222773E-01	.358255E-02
b_1-b_4:	-.423590E+00	-.223744E+00	-.559973E-01	.234539E-02		
A, B, C:	.103422E+01	.202813E+00	-.312452E+00			
Spin Exchange						
a_0-a_5:	.368426E+01	-.177531E+01	-.132486E+01	.377422E-01	.137280E+00	.148016E-01
b_1-b_4:	-.539876E+00	-.288025E+00	.879424E-03	.139590E-01		
A:	.117438E+01					
E = .1585 eV						
Elastic						
a_0-a_5:	.465265E+01	-.183310E+01	-.791552E+00	-.353663E+00	-.208239E-02	.131805E-02
b_1-b_3:	-.388821E+00	-.214909E+00	-.474349E-01			
A, B, C:	.105376E+01	.190445E+00	-.460127E+00			
Spin Exchange						
a_0-a_5:	.354822E+01	-.813437E+00	-.884318E+00	-.240323E+00	-.119994E-01	.797220E-03
b_1-b_4:	-.368145E+00	-.240886E+00	-.398285E-01	-.800510E-04		
A:	.115288E+01					

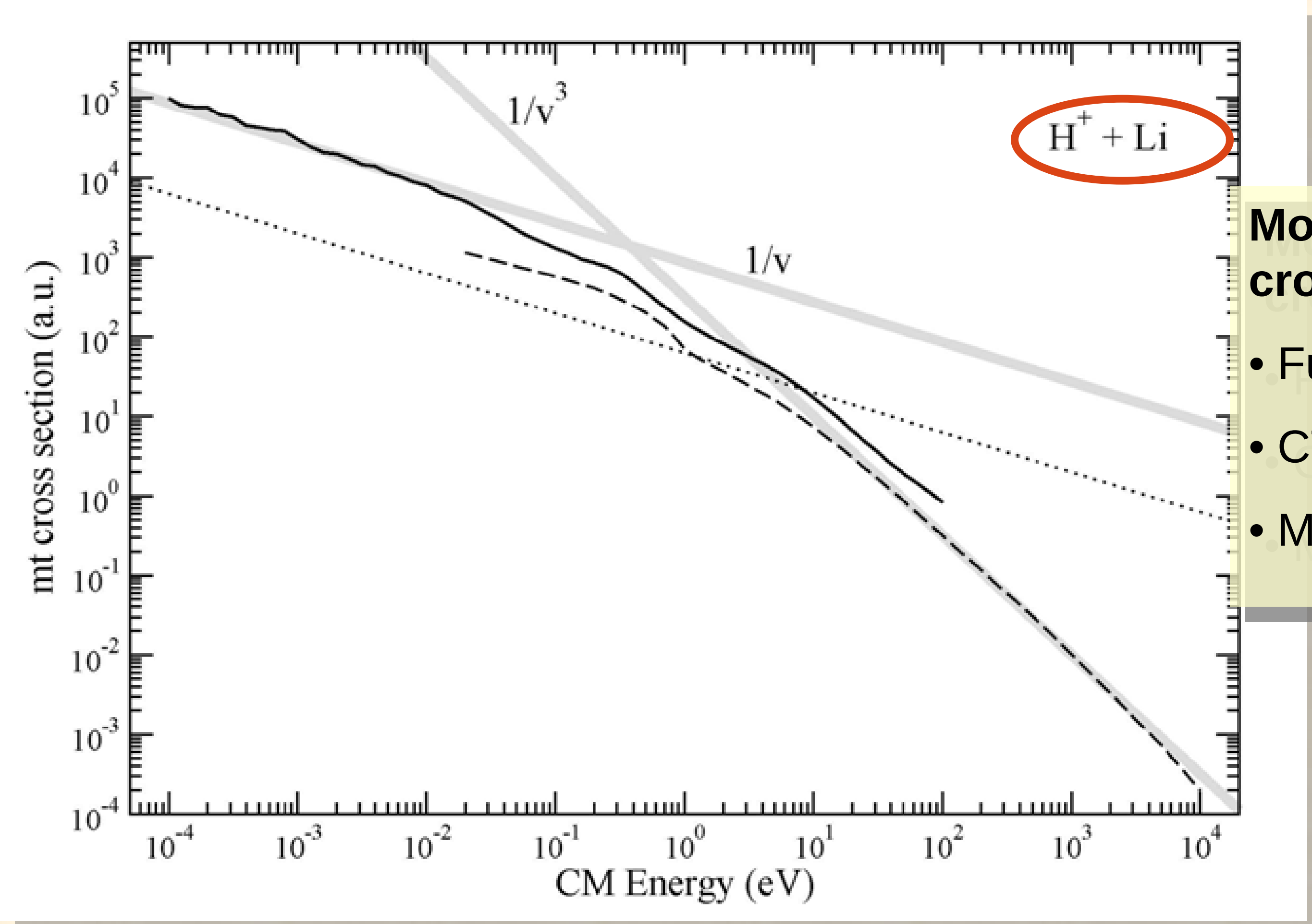
$(H^+,D^+,T^+) + (H,D,T)$	Refs. 12-19
$(H,D,T) + (H,D,T)$	Refs. 12-14, 19, 20
$(H^+,D^+,T^+) + (H_2,D_2,T_2,HD,HT,DT)$	Refs. 13-14, 21
$(H,D,T) + (H_2,D_2,T_2,HD,HT,DT)$	Refs. 13, 22, 23
$H + H_2^+$	Ref. 21
$(H^+,D^+,T^+) + He$	Refs. 13, 19, 24, 25
$(H^+,D^+,T^+) + (Li, Be, B)$	Refs. 32, 33
$(H,D,T) + (Li^+, Be^+, B^+)$	Refs. 32, 33
$(H,D,T) + Li$	Refs. 32, 33
$(H^+,D^+,T^+) + C$	Refs. 24, 26
$(H^+,D^+,T^+) + Ne$	Refs. 24, 25
$(H^+,D^+,T^+) + Ar$	Refs. 24, 25, 27
$(H^+,D^+,T^+) + Kr$	Ref. 24
$(H^+,D^+,T^+) + Xe$	Ref. 24
$(H,H^-,H_2,H_3^+) + H_2$	Compilation of other work in Ref. 12
$(H,D) + He$	Compilation of other work in Ref. 12

Continued work to produced required elastic and related transport cross sections relevant to hydrogen plasmas

Krstic and Schultz, PoP 16, 053503 (2009)

Elastic and transport related data

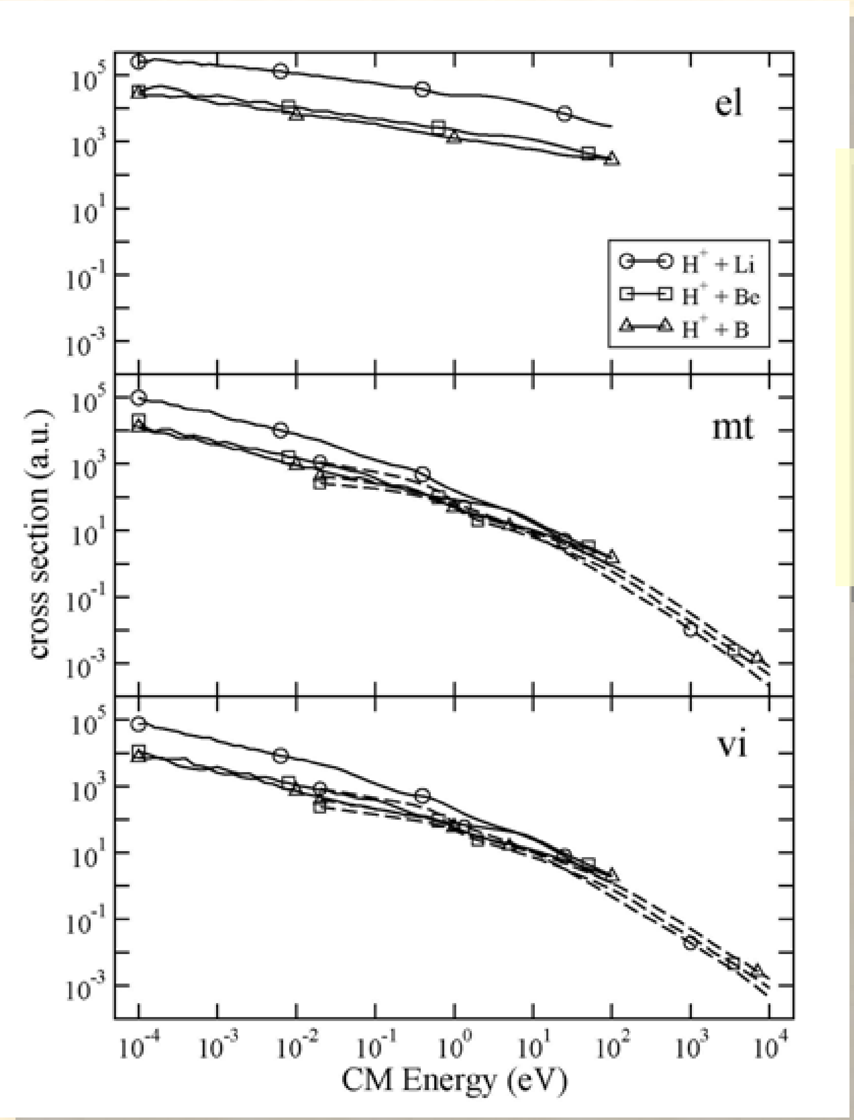
Latest work: Elastic and transport cross sections for neutrals and ions of Li, Be, and B in hydrogen plasmas



Momentum transfer cross section

- Fully QM result
- CTMC result
- Massey-Mohr model

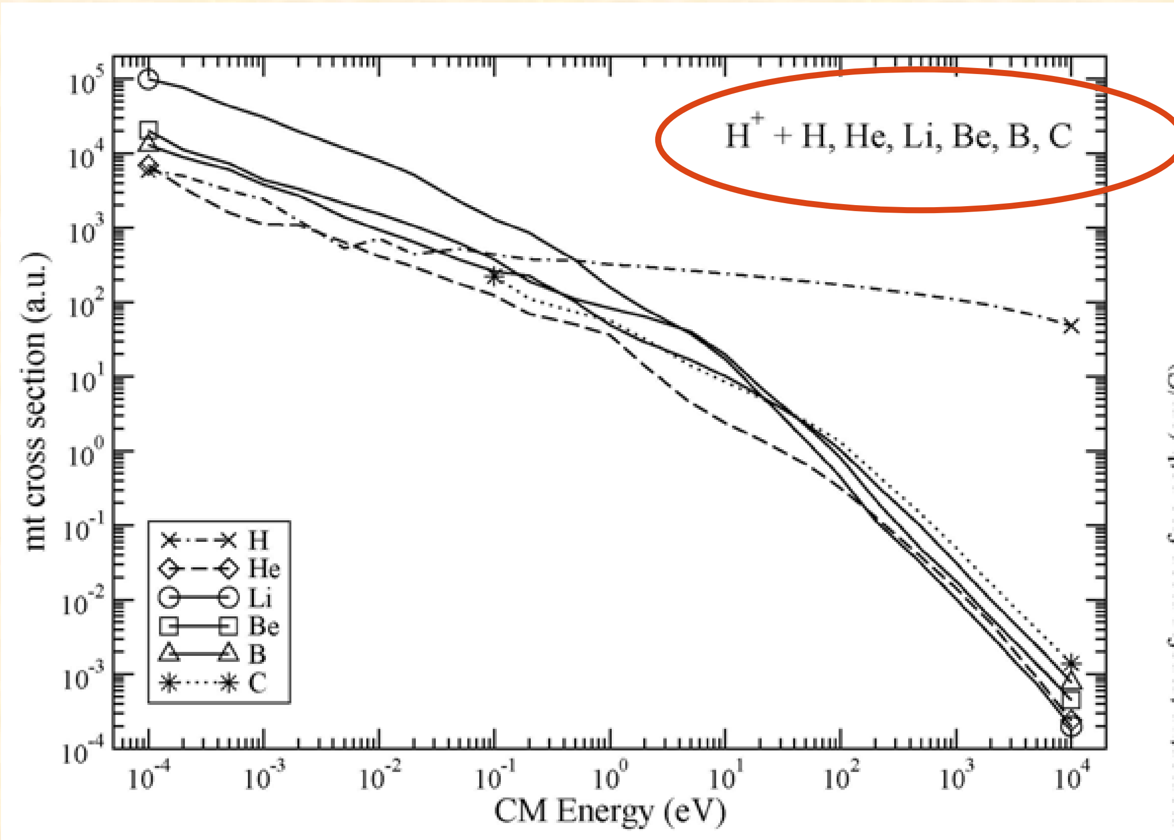
Elastic and transport related data

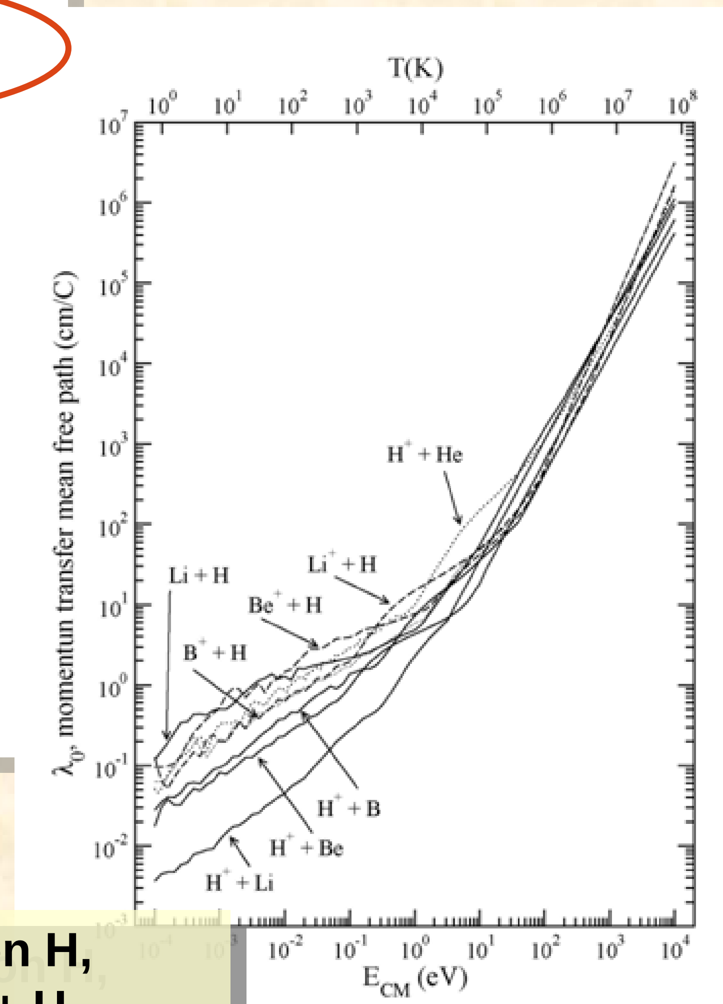


H^+ + Li, Be, and B using QM and CTMC methods

- Elastic scattering cross section (el)
- Momentum transfer cross section (mt)
- Viscosity cross section (vi)

Elastic and transport related data





Momentum transfer cross section for protons colliding with light atoms

Mean free paths for light ions on H, protons on light atoms, and Li + H

Elastic and transport related data

Proposed future work

- First year: H^+ + O, N and O^+,N^+ + H

  ✓ Would complete our calculations for the lightest elements: H, D, T, H_2, He, Li, Be, B, C, N, O, Ne, …

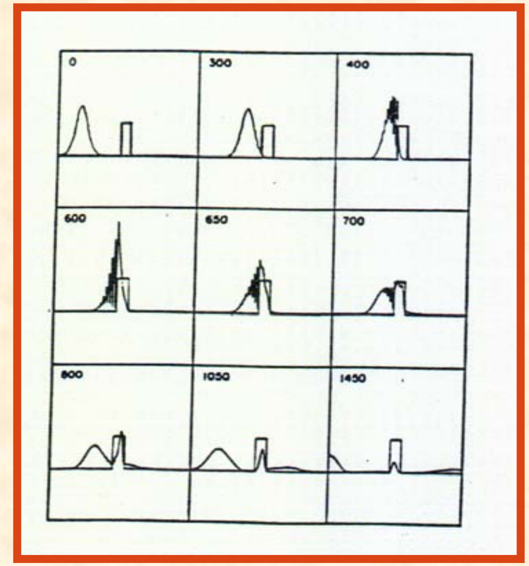
  ✓ O and N are impurities for all plasma facing components exposed to air and nitrogen is a proposed edge/divertor cooling species

- Third year: H^+ + O_2, N_2

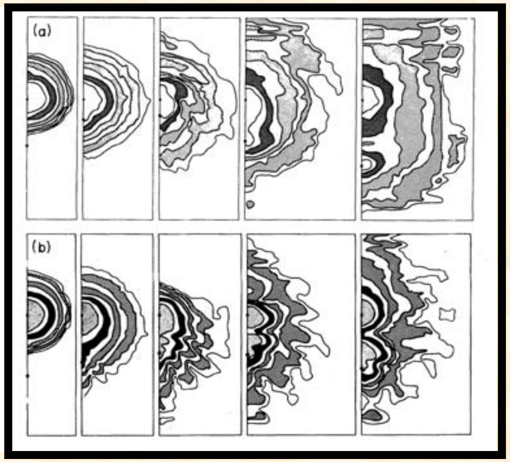
  ✓ First molecular species other than H_2 for us

  ✓ Compare with O, N

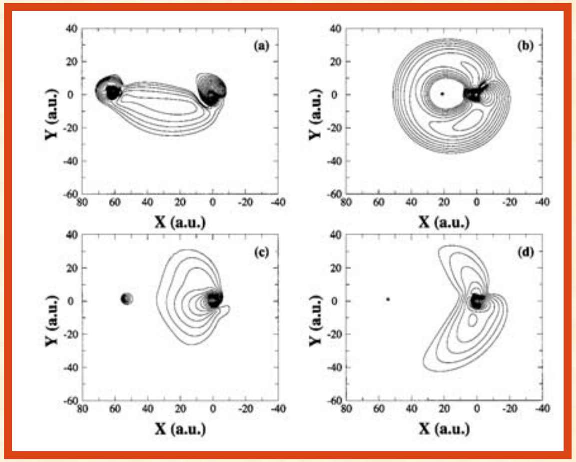
Advancing computational power and numerical techniques for inelastic collisions



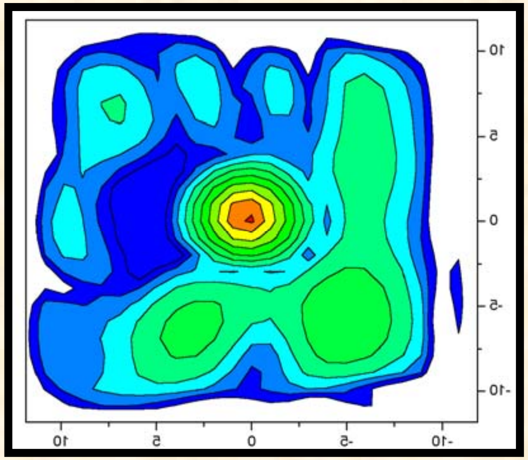
1D, 1960’s
Finite differences, Goldberg, Schey, Schwartz, wavepacket propagation



2D, 1980’s
e.g. low-order finite element approach for H^+, C^{6+} + H

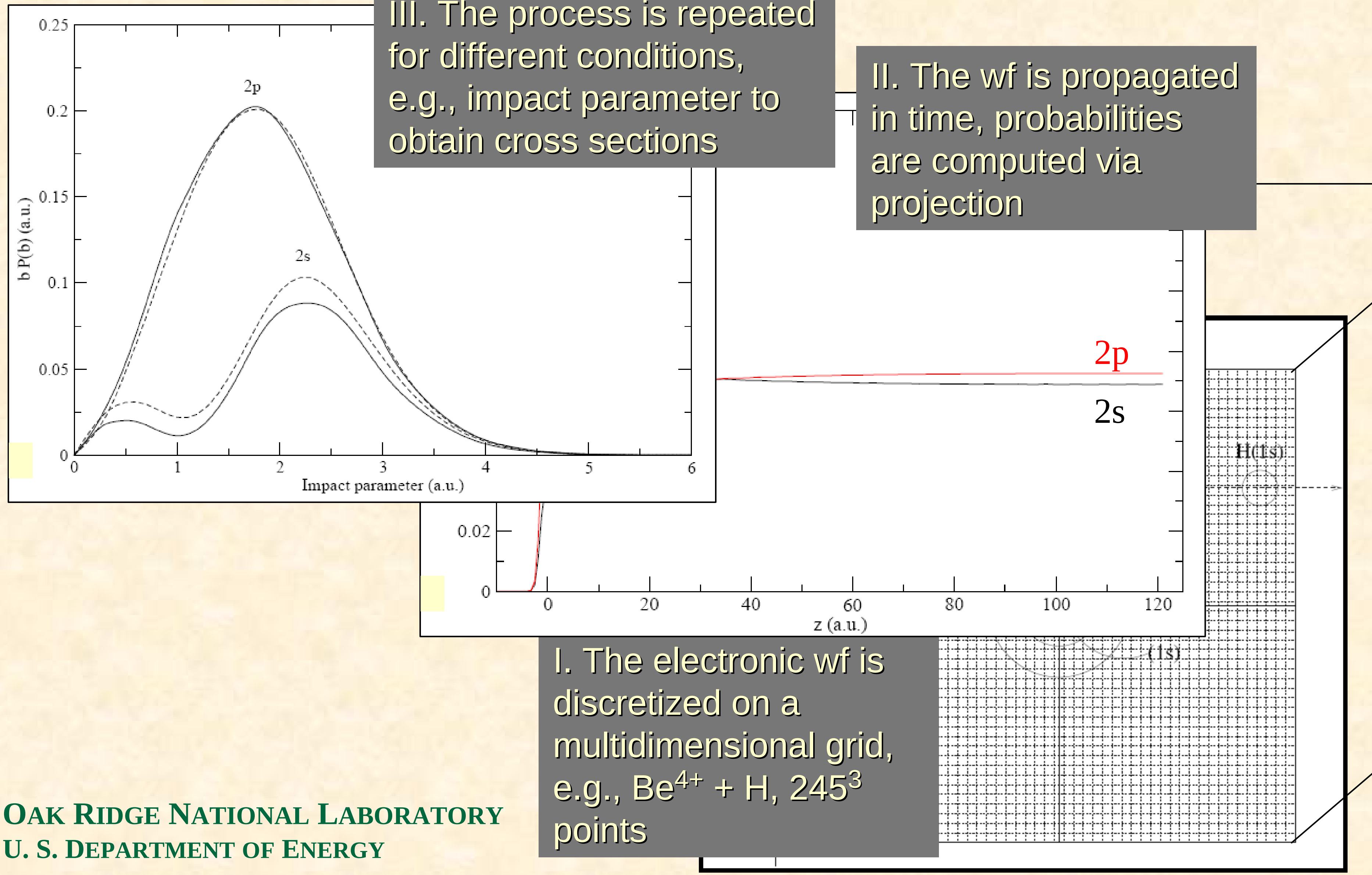


3D, 1990’s
e.g. Basis-spline, Fourier collocation
H^+, p^- + H



3D and up, 2000’s
Non-uniform or adaptive grids, wide variety of discrete representations

The LTDSE method in brief



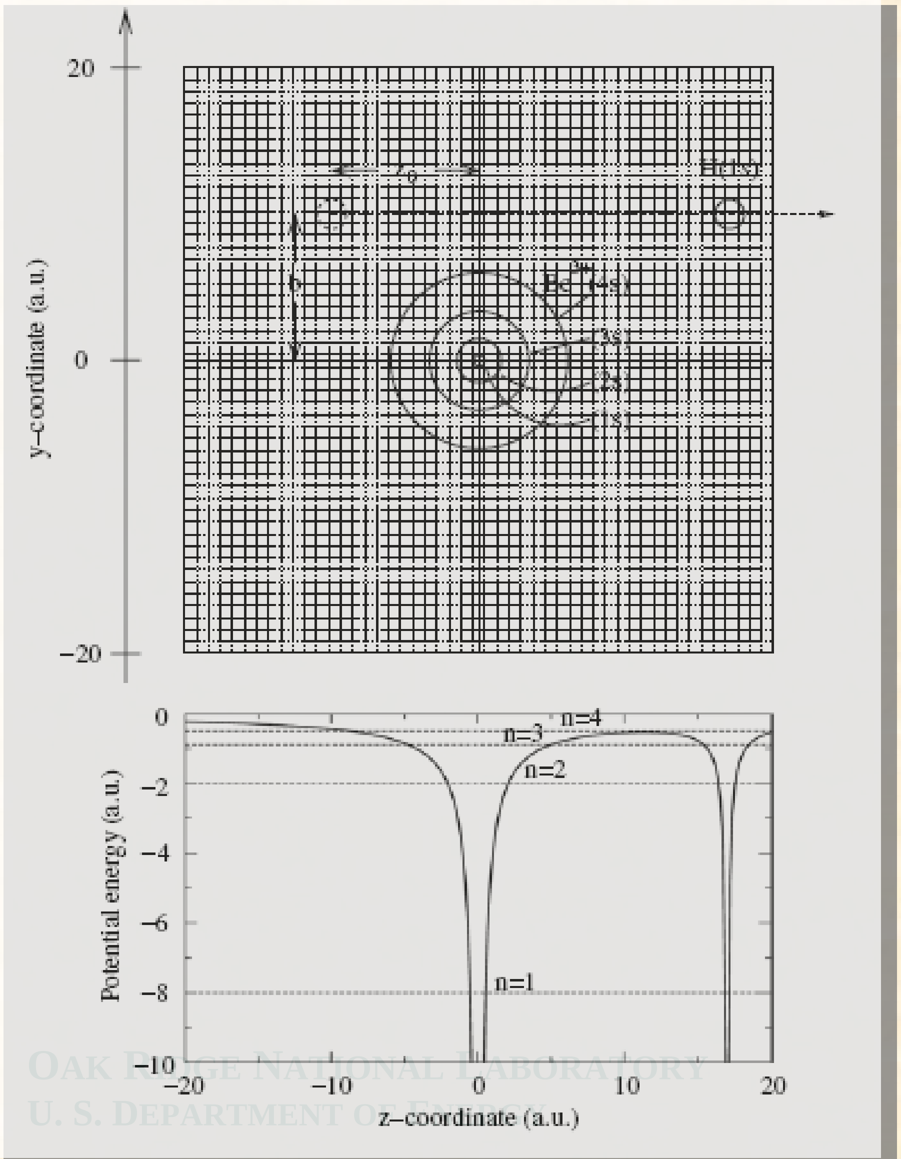
III. The process is repeated for different conditions, e.g., impact parameter to obtain cross sections

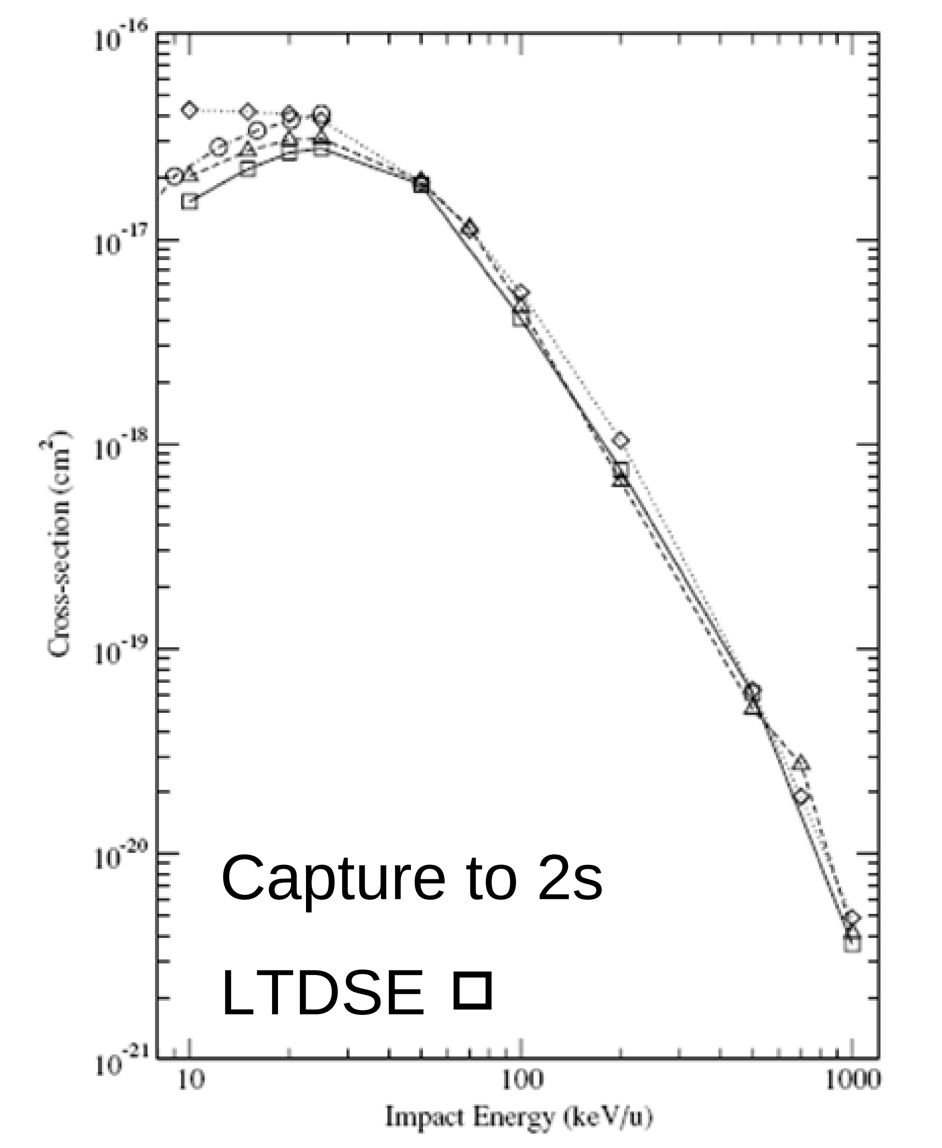
II. The wf is propagated in time, probabilities are computed via projection

I. The electronic wf is discretized on a multidimensional grid, e.g., Be^{4+} + H, 245^3 points

LTDSE for state-selective charge transfer in Be^{4+} + H collisions

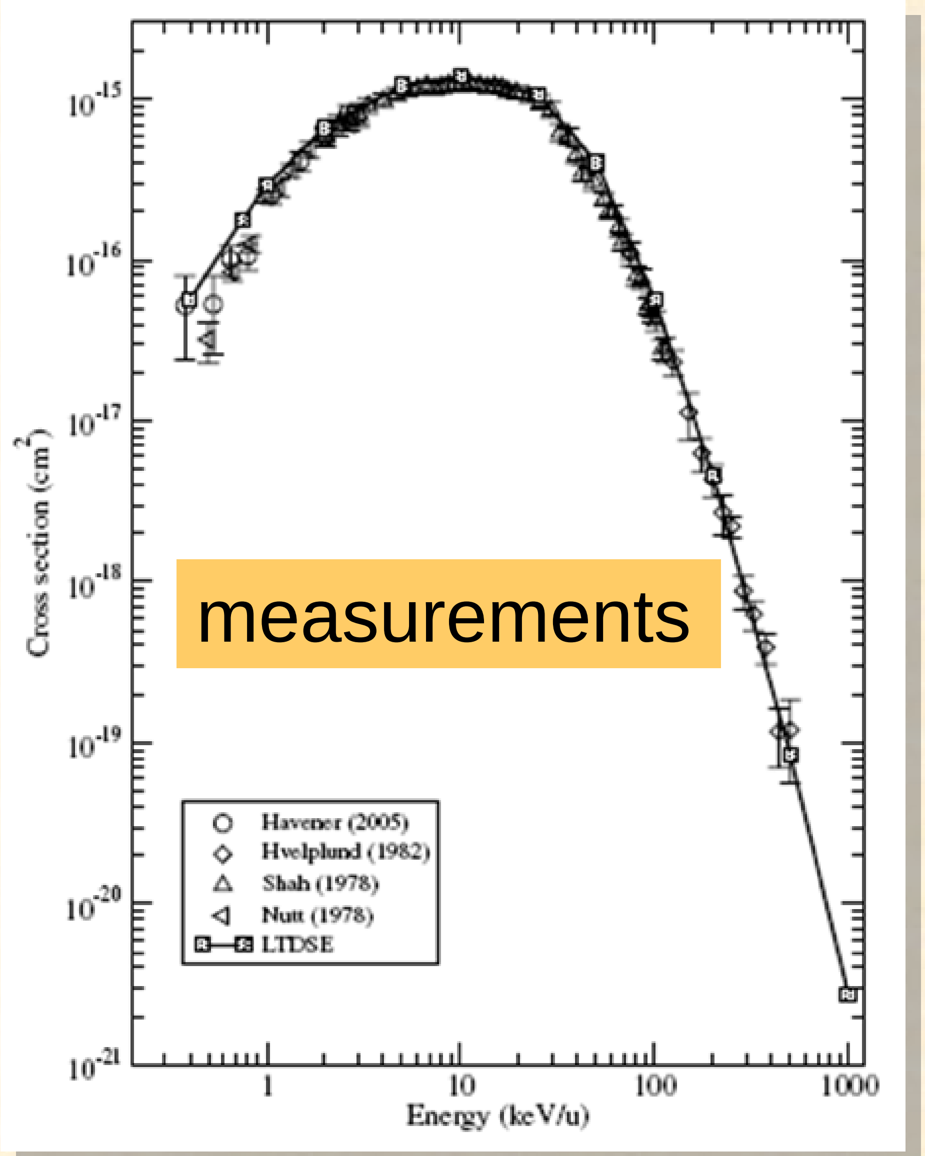
Minami, Pindzola, Lee, Schultz, JPB 2006

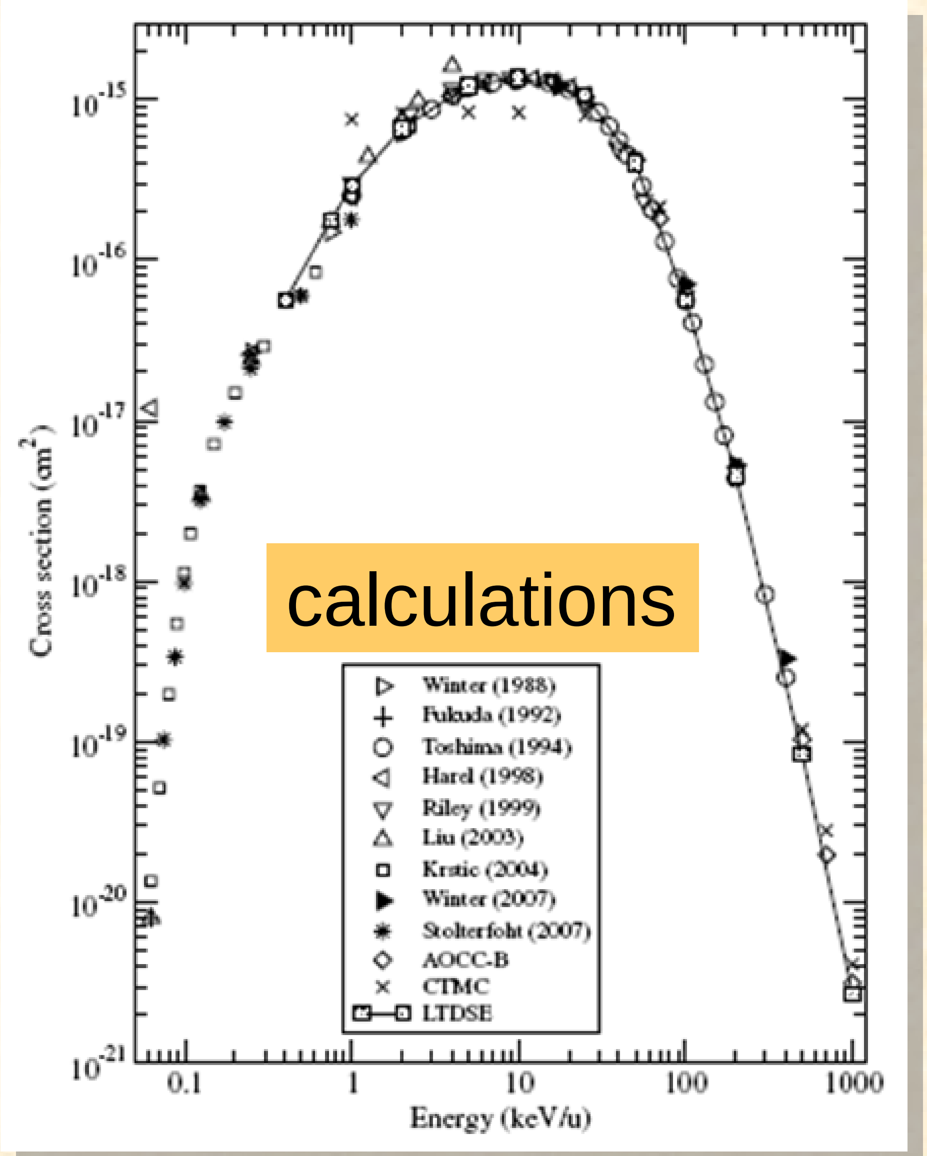




LTDSE for state-selective charge transfer in He^{2+} + H collisions

Minami, Lee, Pindzola, Schultz, JPB 2008





LTDSE for state-selective charge transfer in He^{2+} + H collisions

Minami, Lee, Pindzola, Schultz, JPB 2008

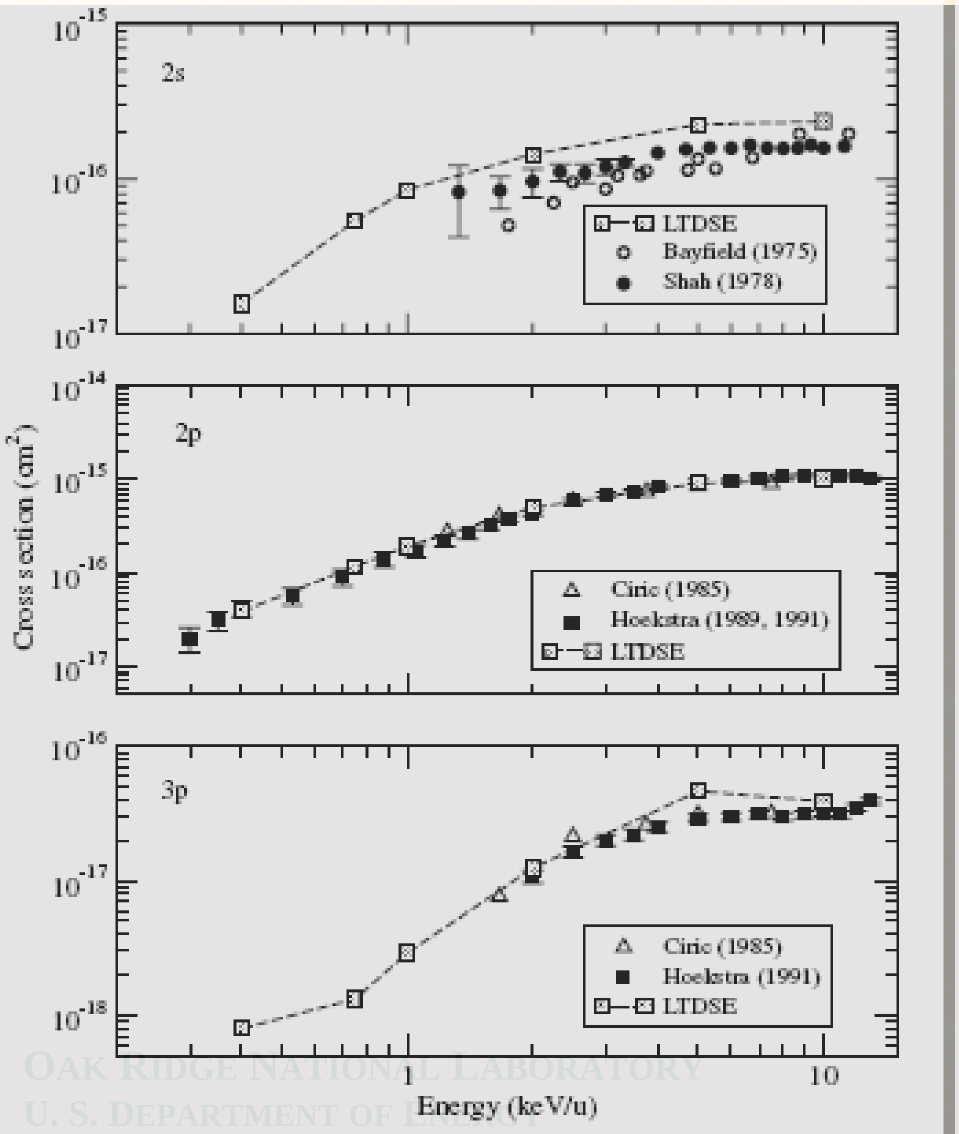
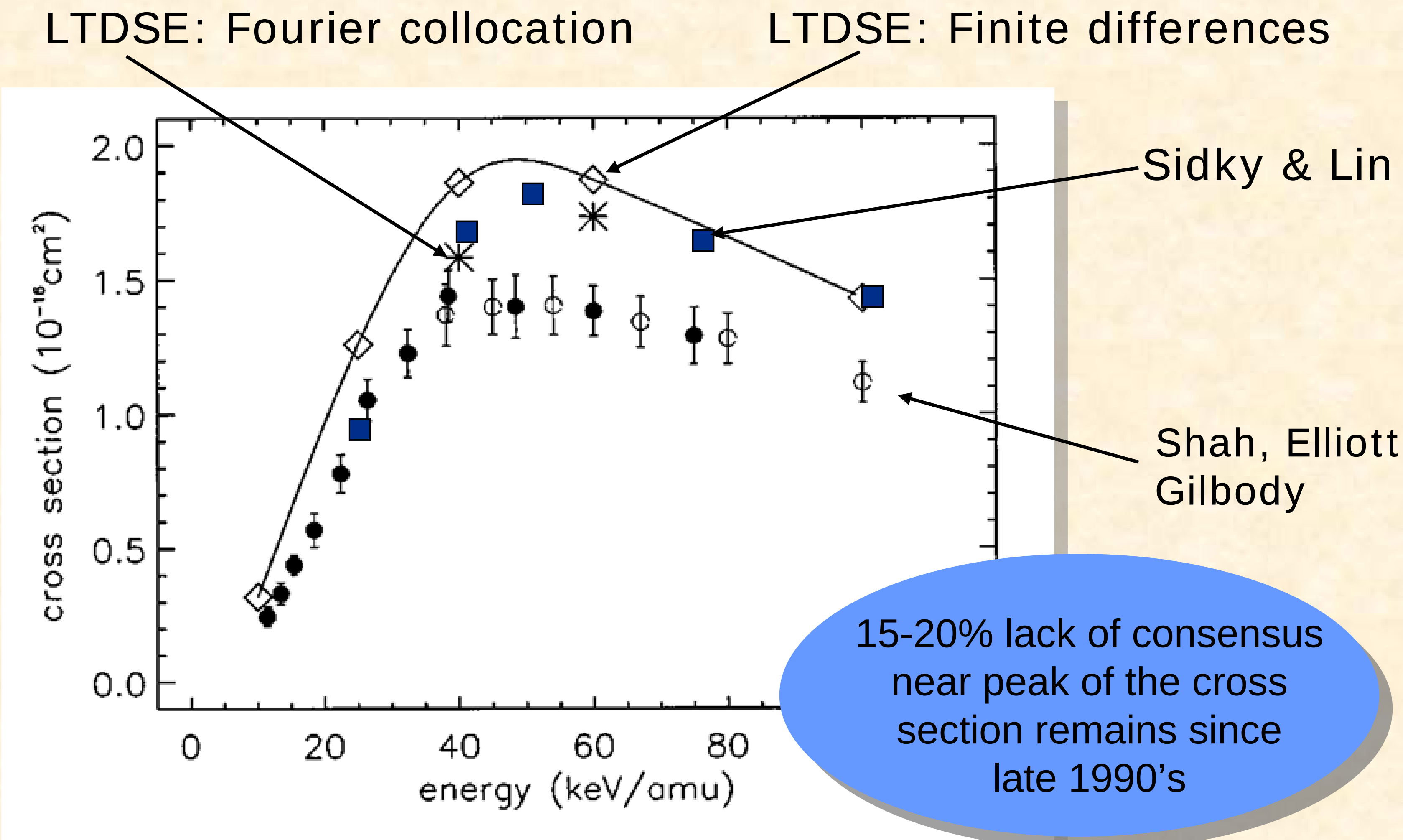


Table A6. State-selective cross sections (in cm^2) for charge transfer in 50 keV/u He^{2+} + H collisions.

n, l	LTDSE	AOCC-A	AOCC-B	CTMC
1	2.15(−17)	2.34(−17)	2.37(−17)	2.72(−17)
2, 0	4.89(−17)	4.97(−17)	4.93(−17)	3.93(−17)
2, 1	1.46(−16)	1.44(−16)	1.45(−16)	1.99(−16)
2	1.95(−16)	1.94(−16)	1.94(−16)	2.38(−16)
3, 0	2.72(−17)	2.65(−17)	3.15(−17)	2.10(−17)
3, 1	4.57(−17)	4.28(−17)	4.45(−17)	6.14(−17)
3, 2	1.19(−17)	1.11(−17)	1.20(−17)	6.39(−18)
3	8.48(−17)	8.04(−17)	8.80(−17)	8.88(−17)
4	3.58(−17)	3.88(−17)	4.23(−17)	3.55(−17)
5	2.41(−17)	2.61(−17)	2.36(−17)	1.75(−17)
6				9.95(−18)
7				6.16(−18)
8				4.08(−18)
9				2.85(−18)
10				2.06(−18)
11				1.55(−18)
12				1.18(−18)
13				9.34(−19)
14				7.47(−19)
15				6.07(−19)
16				4.94(−19)
17				4.15(−19)
18				3.52(−19)
19				2.97(−19)
20				2.56(−19)
$\sigma(n = 1\text{–}5)$	3.61(−16)	3.62(−16)	3.72(−16)	4.07(−16)
$\sigma(n = 1\text{–}20)$	4.05(−16)	4.10(−16)	4.15(−16)	4.39(−16)

Ionization of atomic hydrogen by proton impact

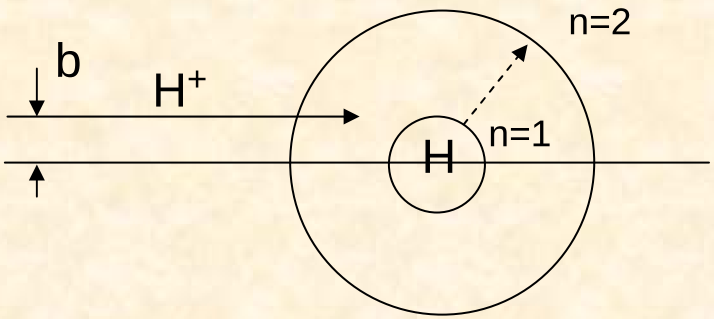


15-20% lack of consensus near peak of the cross section remains since late 1990's

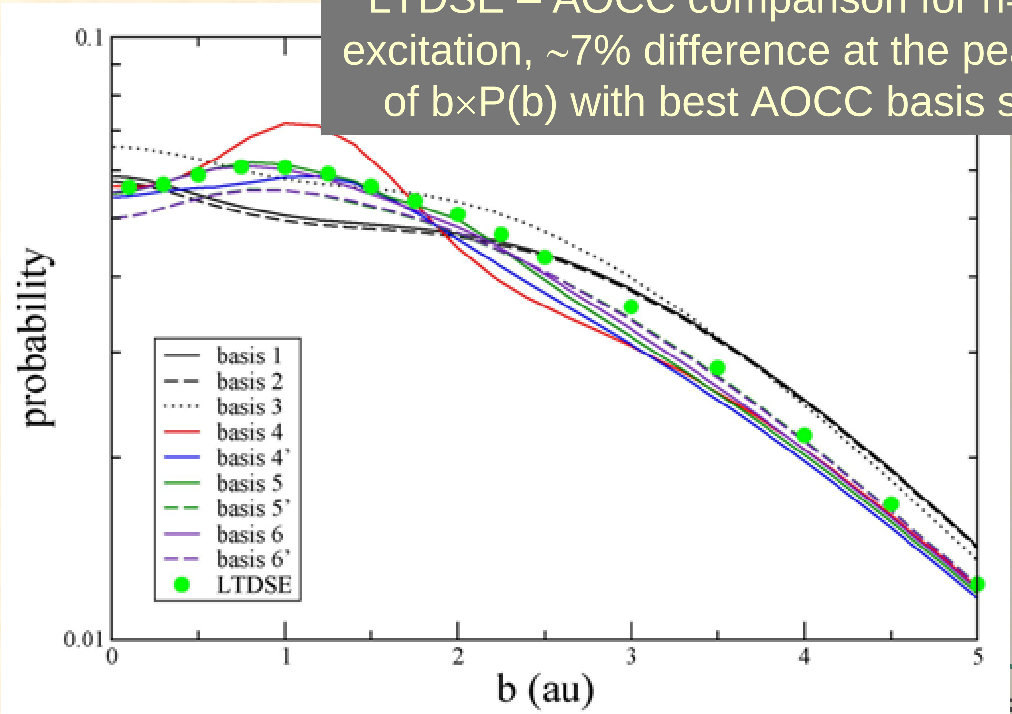
Ionization of atomic hydrogen by proton impact

The LTDSE method allows each aspect of the calculation to be improved to demonstrate convergence to within a desired level of precision

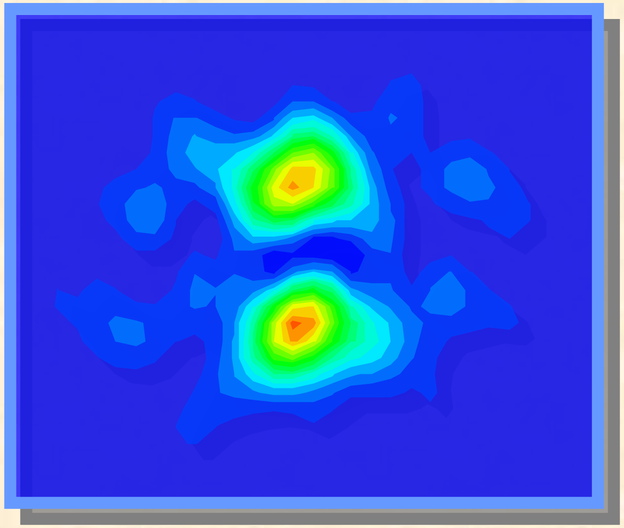
- Use highest order derivative representation
- Use time steps small enough that error in time propagator is insignificant
- Separate calculation of each n-level for target- and projectile-centered state to set box size, compute for enough n-levels to reach known scaling
- Demonstrate convergence of results with initial and final internuclear separation
- Demonstrate convergence with mesh spacing



LTDSE – AOCC comparison for n=2 excitation, ~7% difference at the peak of b×P(b) with best AOCC basis set

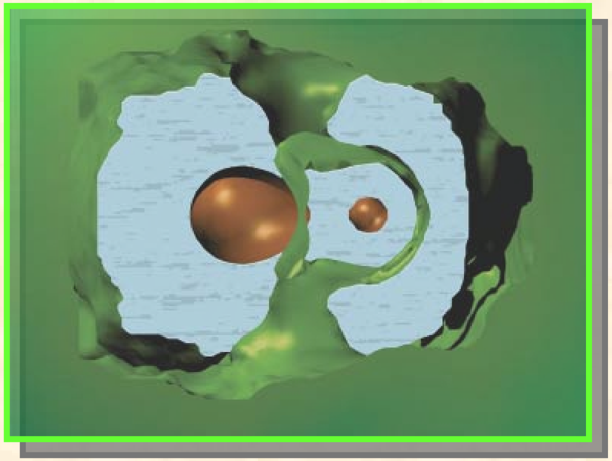


Ionization of atomic hydrogen by proton impact



Complementary to advancing experimental techniques such as the reaction microscope, LTDSE and other contemporary methods are driving significantly increased accuracy of results

and these developments go hand in hand with discovery and elucidation of few-body quantum dynamics



A very recent discovery has been that vortices appear in the electronic wavefunction during ion-atom collisions,

• that they should be observable in experiments,

• that they could play a significant role in angular momentum transfer not previously recognized, and

• that they are quite likely ubiquitous

Macek, Sternberg, Ovchinnikov, Lee, Schultz, PRL 2009

Inelastic collision data

Proposed future work

- First year: H^+,C^{6+} + H excitation of n=2,3, … substates

  ✓ For beam diagnostics, beam emission and motional Stark effect measurements, derived plasma parameters

- Second-third year: H^+ + H

  ✓ Benchmark ionization total cross section across a broad range of eneriges