Physique des Infinis
Une Initiative Sorbonne Université

# Modeling iodine plasma for electric propulsion

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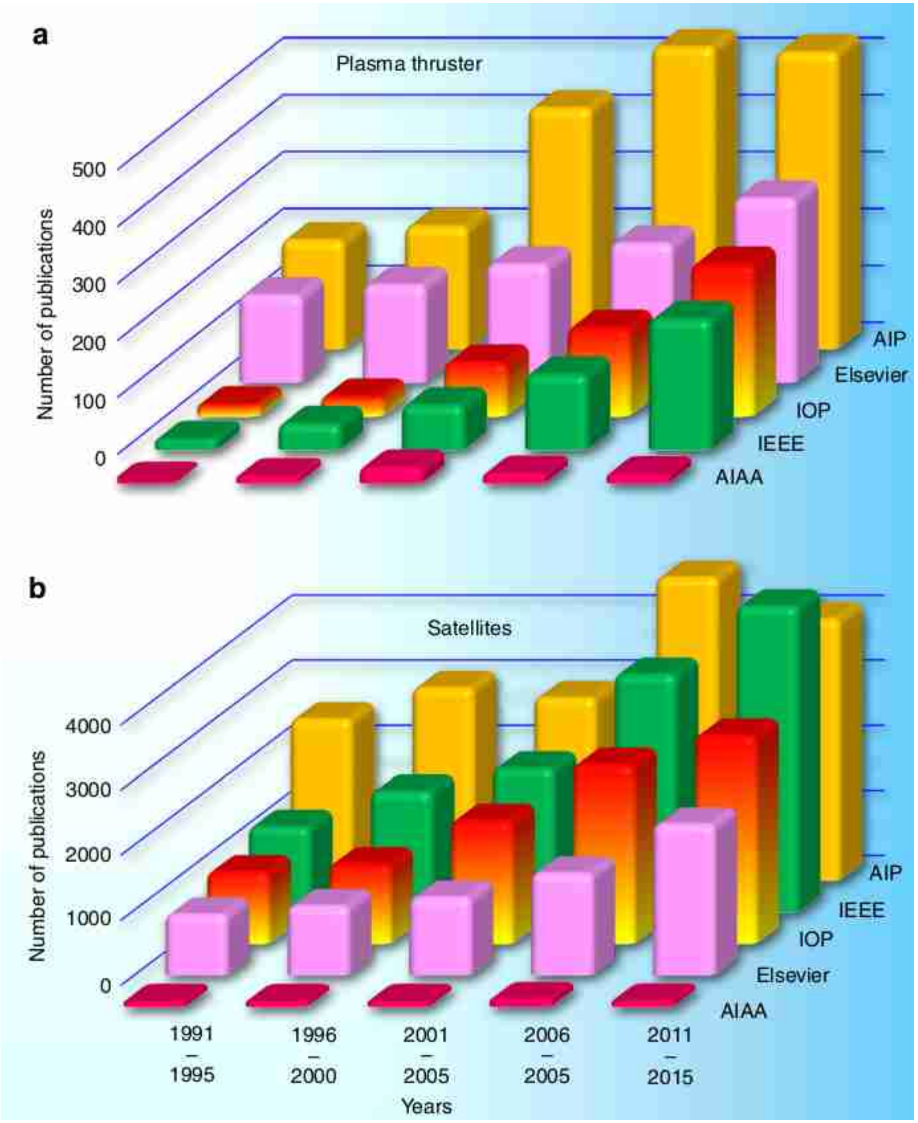
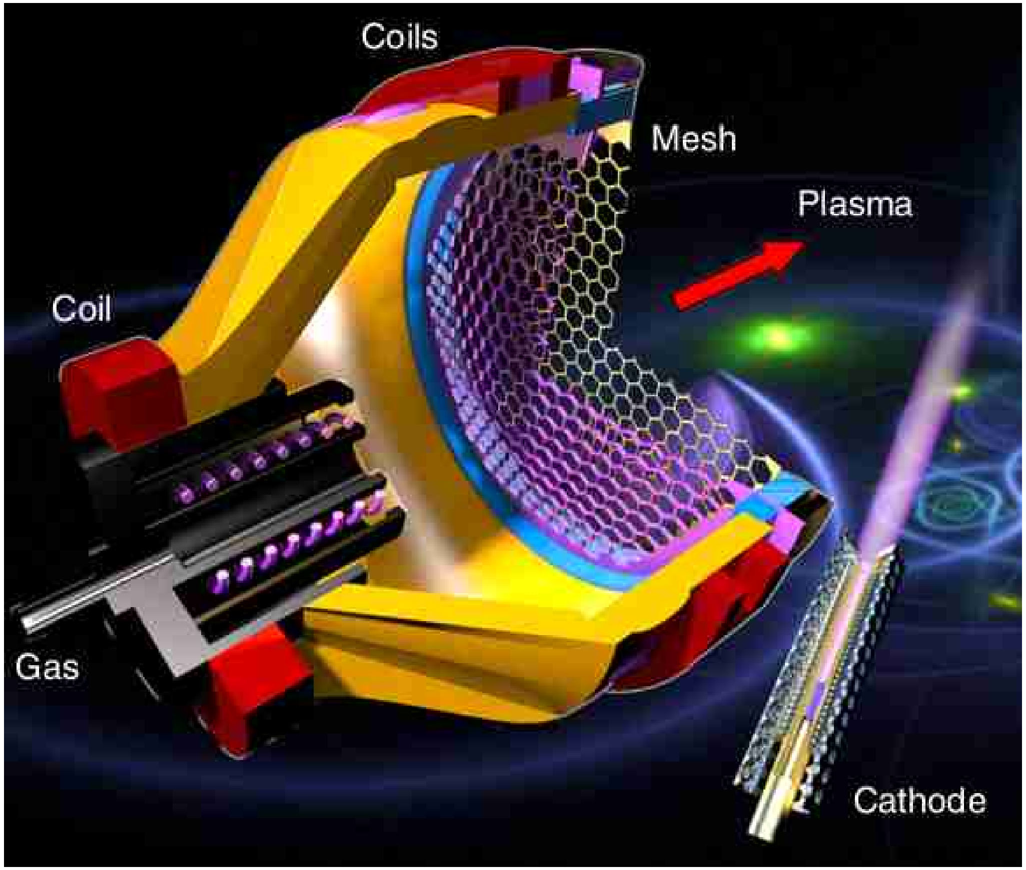
# Plasma for electric propulsion

Photo illustration of satellites surrounding earth
MS. TECH: ORIGINAL IMAGES: NASA




Review Article in Nat. Comm. 9, 879 (2018).

# Plasma for electric propulsion




$$F = \frac{\mathcal{W}}{\mathcal{E}_{\text{ion}} + e\Delta\phi}\left(2e\Delta\phi m_i\right)^{1/2}$$

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# Plasma for electric propulsion

## Xenon

High mass (131.3 amu)
Low IP (12.1 eV)

Rare
Expensive
Gaz

## Iodine ($I_2$)

High mass (253.8 amu)
Low IP (9.3 eV)
Solid
Cheap

Richer “chemistry”
Scarce database

# Plasma for electric propulsion

SPACENEWS



## French startup demonstrates iodine propulsion in potential boost for space debris mitigation efforts

by **Andrew Jones** — January 22, 2021

ThrustMe's NPT30-I2-1U propulsion system installed on the Spacety Beihanghongshi-1 CubeSat. Credit: Spacety

THRUSTME

# Objectives

## Provide the most complete description of Iodine Plasma

* Set-up a (complete) global model
* Validate the model (compare to experiments)
* Rich and accurate database
  (reactions in volume and at the walls)

* Performance of iodine thrusters

# Global Model

Reactions rates
(neutralization,
recombination,
charge transfer,...)

Initial conditions
(Gas pressure, power, …)

$$\frac{\mathrm{d}n_k}{\mathrm{d}t} = \sum_j \left\{ (a_{kj}^{(2)} - a_{kj}^{(1)}) k_j \prod_l n_l^{a_{lj}^{(1)}} \right\}$$

$$\frac{d}{dt}\left(\frac{3}{2} e n_e T_e\right) = P_{abs} - P_{loss}$$

Densities
Temperatures

Performance

# Current status

## LPP0D Code

$I_2$, $I$, $I_2^+$, $I^+$, $I^-$, $e^-$

| Reaction | Process | Threshold [eV] | Model | Reference |
|---|---|---|---|---|
| *Electron impact I* | | | | |
| $I + e^- \rightarrow I + e^-$ | Elastic | 0 | 0D+PIC | [74] |
| $I + e^- \rightarrow I + 2e^-$ | Ionization | 11.64 | 0D+PIC | [74] |
| $I + e^- \rightarrow I^* + e^-$ | Excitation | 0.9529 | 0D+PIC | [74] |
| *Electron impact* $I_2$ | | | | |
| $I_2 + e^- \rightarrow I_2 + e^-$ | Elastic | 0 | 0D+PIC | [74] |
| $I_2 + e^- \rightarrow I_2^+ + 2e^-$ | Ionization | 9.31 | 0D+PIC | [74] |
| $I_2 + e^- \rightarrow I^+ + I + 2e^-$ | Dissociative ionization | 10.75 | 0D+PIC | [74] |
| $I_2 + e^- \rightarrow I^- + I$ | Dissociative attachment | 0 | 0D+PIC | [74] |
| $I_2 + e^- \rightarrow 2I + e^-$ | Dissociation | 1.567 | 0D+PIC | [74] |
| *Electron impact dissociation of* $I_2^+$ | | | | |
| $I_2^+ + e^- \rightarrow I^+ + I + e^-$ | Dissociation | 2.17 | 0D | [75] |
| *Electron detachment from* $I^-$ | | | | |
| $I^- + e^- \rightarrow I + 2e^-$ | Detachment | 2.1768 | 0D | [75] |
| *Recombination* | | | | |
| $I^- + I_2^+ \rightarrow I + I_2$ | Mutual neutralization | 0 | 0D+PIC | [69] |
| $I^- + I^+ \rightarrow 2I$ | Mutual neutralization | 0 | 0D+PIC | [158] |
| *Isotropic scattering of ions* | | | | |
| $I + I^+ \rightarrow I + I^+$ | Elastic | 0 | PIC | Langevin |
| $I + I_2^+ \rightarrow I + I_2^+$ | Elastic | 0 | PIC | Langevin |
| $I + I^- \rightarrow I + I^-$ | Elastic | 0 | PIC | Langevin |
| $I_2 + I^+ \rightarrow I_2 + I^+$ | Elastic | 0 | PIC | Langevin |
| $I_2 + I_2^+ \rightarrow I_2 + I_2^+$ | Elastic | 0 | PIC | Langevin |
| $I_2 + I^- \rightarrow I_2 + I^-$ | Elastic | 0 | PIC | Langevin |
| *Backscattering of ions* | | | | |
| $I + I^+ \rightarrow I^+ + I$ | Charge exchange | 0 | PIC | [124] |
| $I + I^- \rightarrow I^- + I$ | Charge exchange | 0 | PIC | [124] |
| $I_2 + I_2^+ \rightarrow I_2^+ + I_2$ | Charge exchange | 0 | PIC | [53] |
| $I_2 + I^+ \rightarrow I_2^+ + I$ | Charge exchange | 0 | 0D+PIC | [124]+[81] |
| *Surface recombination* | | | | |
| $I \rightarrow \frac{1}{2}I_2$ | Wall process | 0 | 0D+PIC | [47] |

Table 5.2: Reactions of a low temperature iodine plasma investigated in this work.

Romain Lucken's PhD thesis (LPP, 2019).

# Current status

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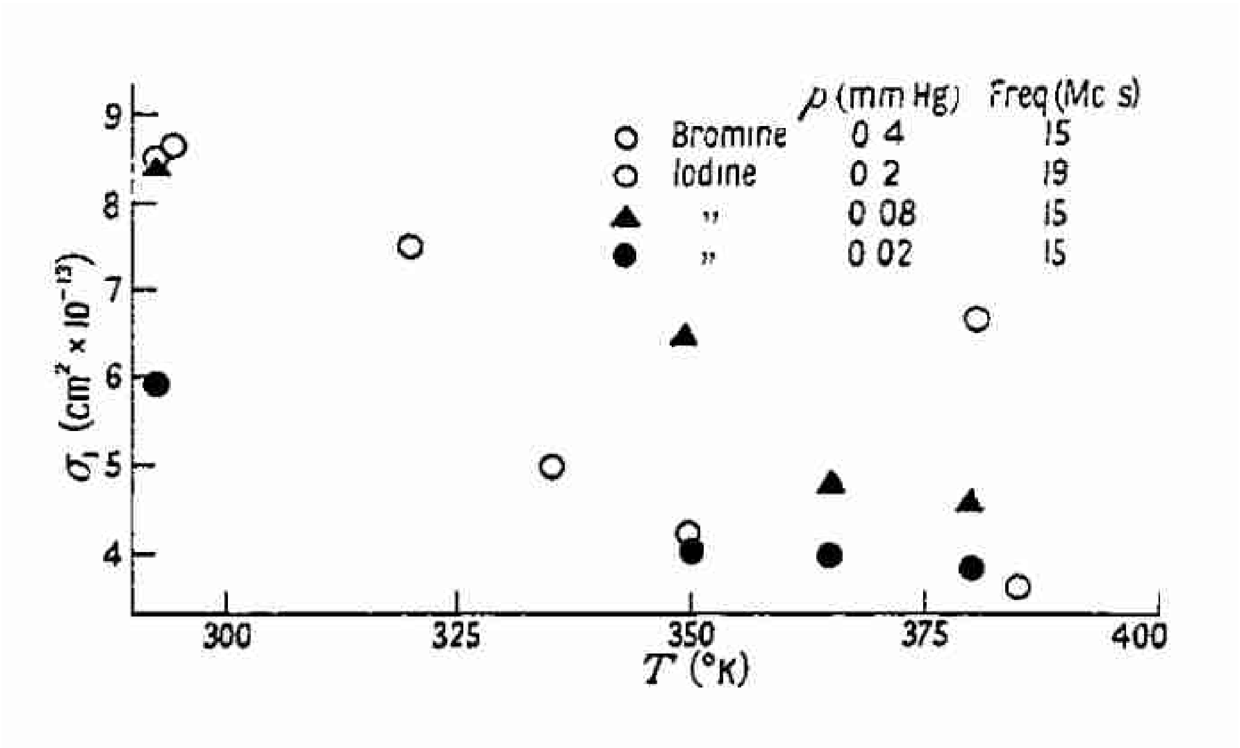
# Ab initio collision cross sections

## Mutual Neutralization

**$I^+ - I^- \Rightarrow I - I$**

In [158] (Yeung et al. (1957)), cross sections were estimated from the afterglow plasma of a highly electronegative gas discharge



# $I_2$ molecule

Importance of spin-orbit coupling in $I_2$

We use relativistic electronic structure calculations :
Dirac software

P rogram
• for
A tomic
• and
M olecular

D irect
I terative
R elativistic
A ll-electron
C alculations

Instead of solving the Schrödinger Equation

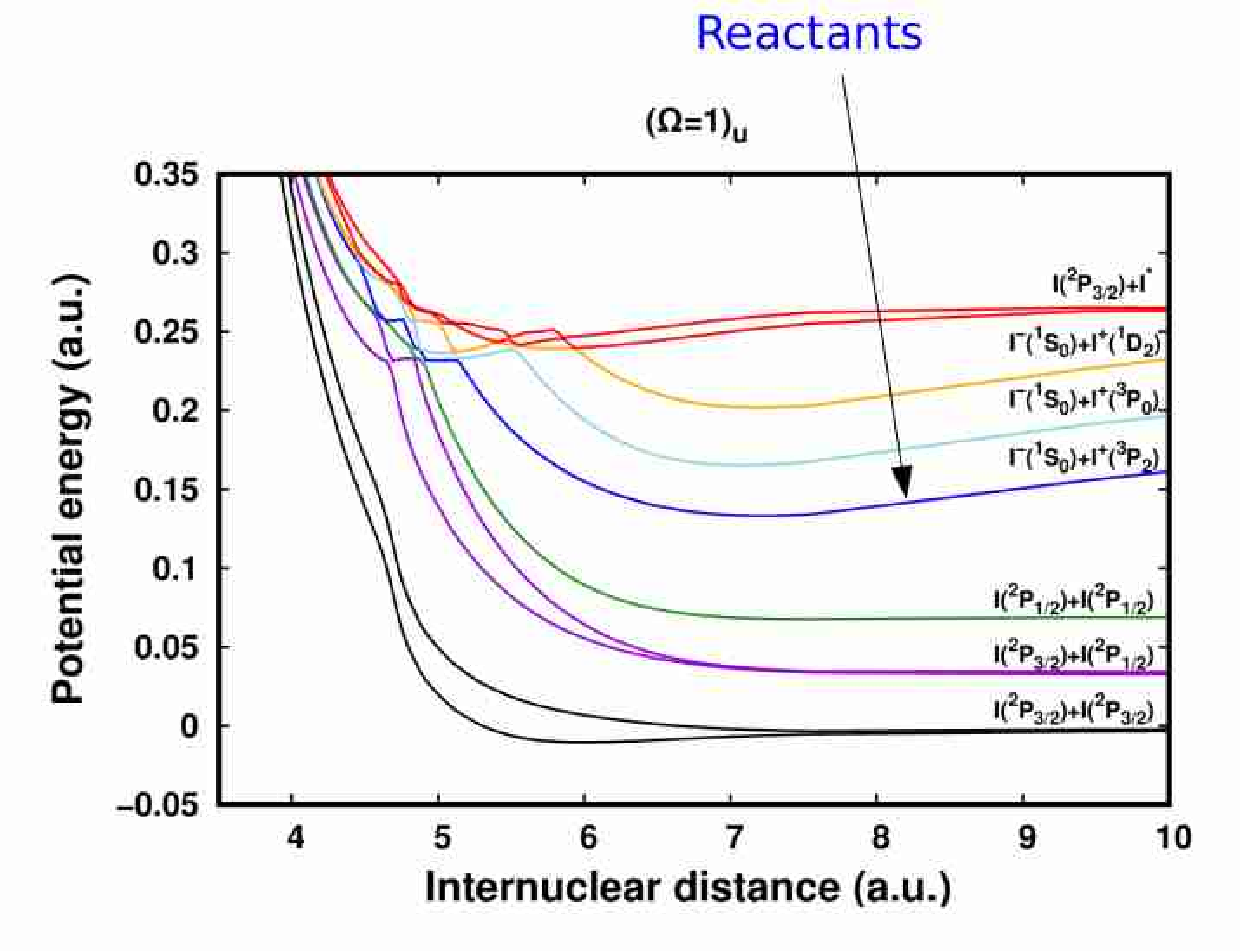
We solve the Dirac equation

Methods :

- 4-componant Dirac Hartree Fock (DHF)
- Multi-reference Configuration interaction (MRCI)

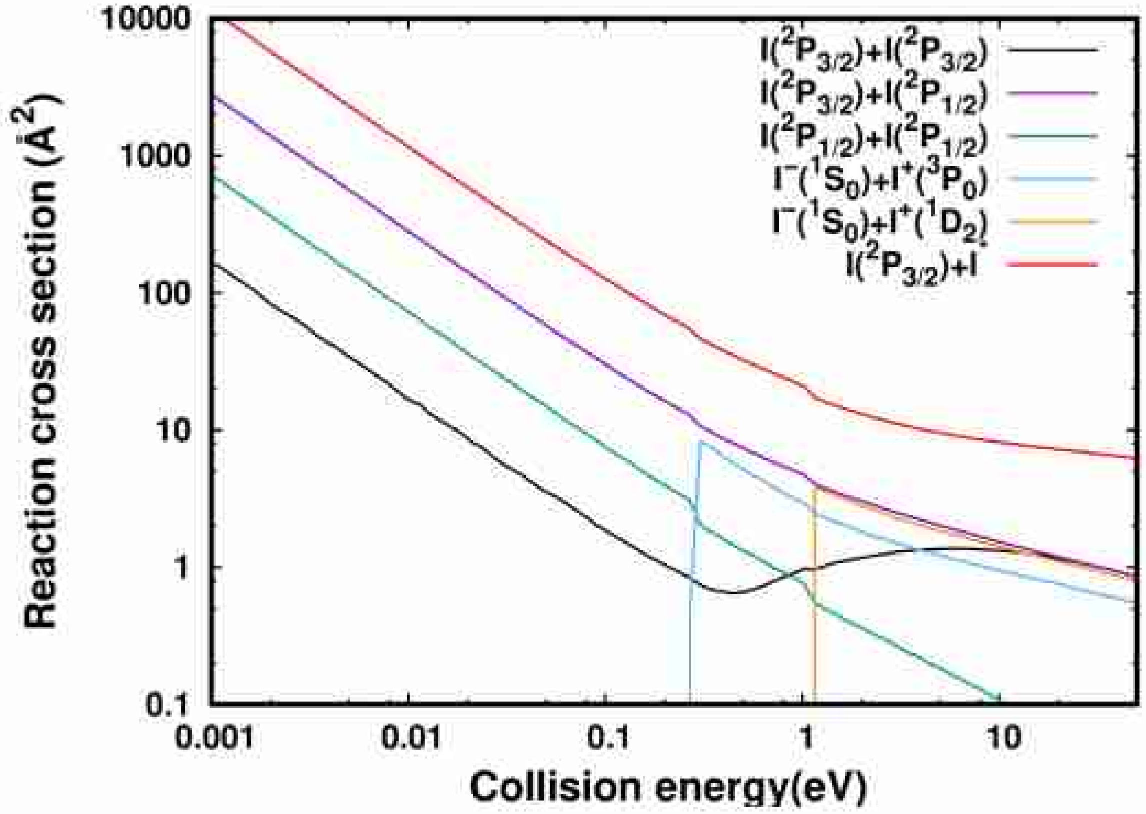
PEC computed by X. Yuan
(Phlam Laboratory)

# $I_2$ molecule



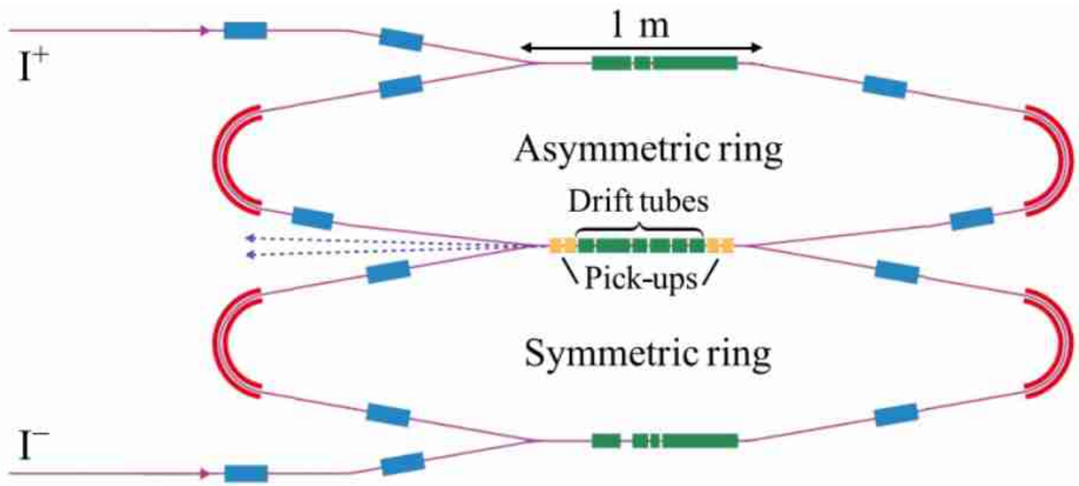
Reactants
(Ω=1)u
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
−0.05
Potential energy (a.u.)
4
5
6
7
8
9
10
Internuclear distance (a.u.)
I(²P3/2)+I*
I⁻(¹S0)+I⁺(¹D2)
I⁻(¹S0)+I⁺(³P0)
I⁻(¹S0)+I⁺(³P2)
I(²P1/2)+I(²P1/2)
I(²P3/2)+I(²P1/2)
I(²P3/2)+I(²P3/2)

# Ab initio collision cross sections




Can we check the accuracy of our cross sections?

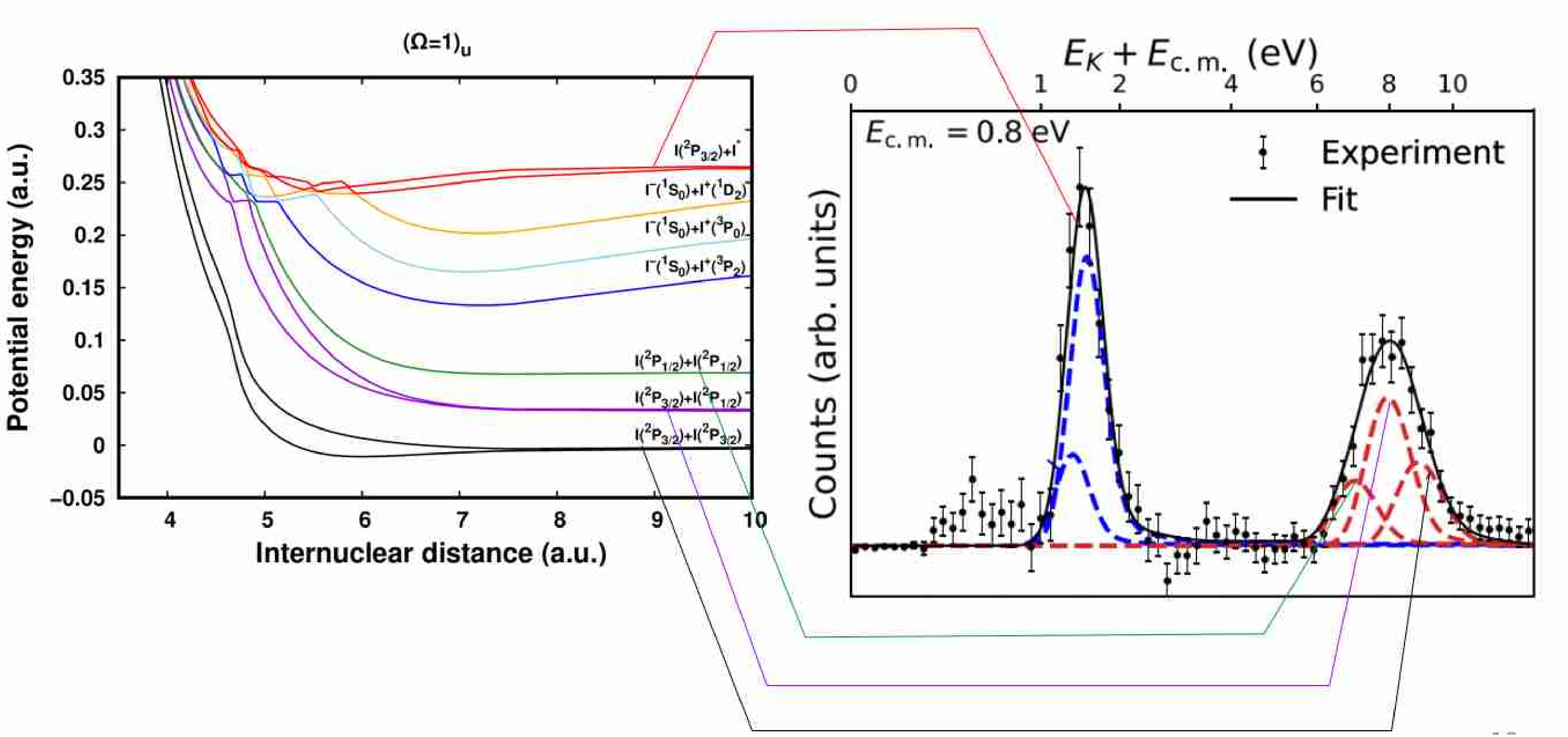
# Expt. @ DESIREE




Collision energies :

- 0.1 eV
- 0.8 eV

# Expt. @ DESIREE



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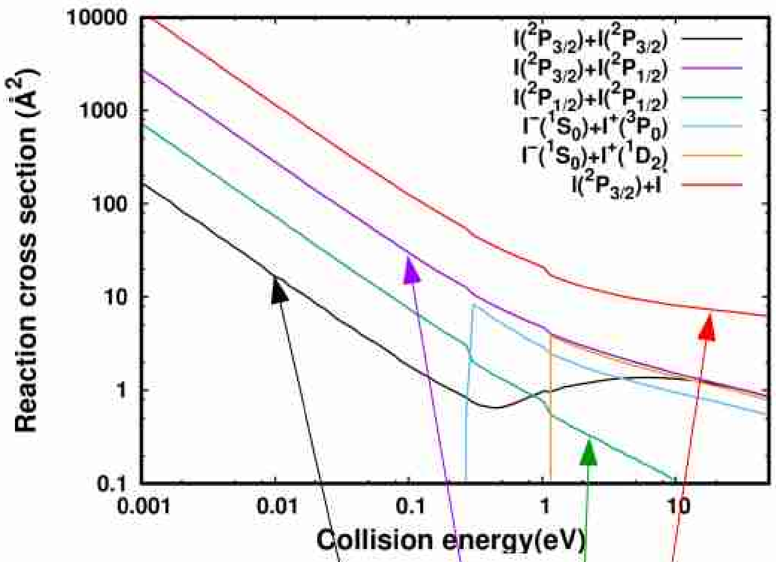
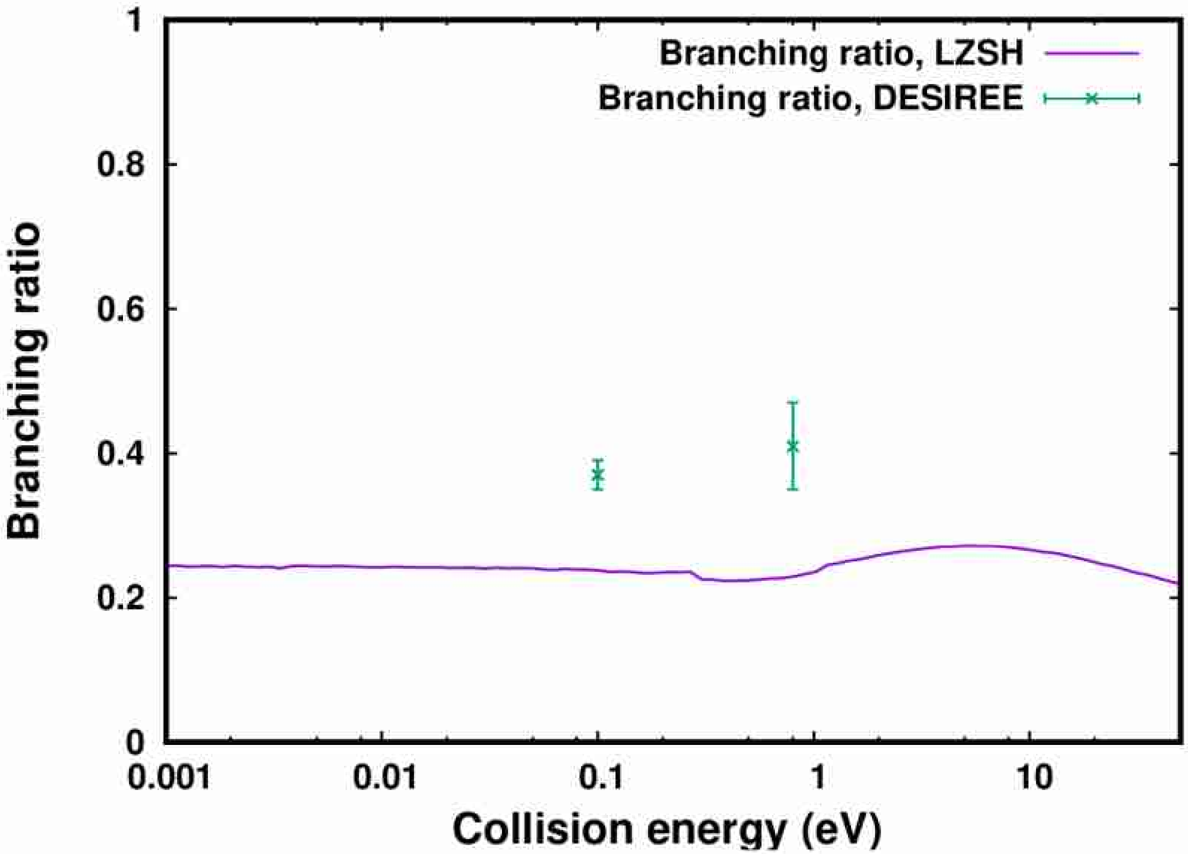



$$BR = \frac{\sigma_1 + \sigma_2 + \sigma_3}{\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4}$$



# Next Steps

* Add more species in the model

* Add more reactions in the model
  ($I^-$ + $I_2^+$, Theory and Expt.)

* Compute/revise reactions rates

* Check the accuracy of the data/model
  => Validate the model + Study of performance

# Acknowledgments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Thank you for your attention