# Rotational transitions induced by collisions of $H_2^+$ ions with low energy electrons


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## Abstract

Electron-impact dissociative recombination(1), ro-vibrational (de-)excitation (2) of molecular cations play a major role in the kinetics and energy balance of

$$AB^+(N_i^+, v_i^+) + e^- \rightarrow A + B \quad (1) \qquad AB^+(N_i^+, v_i^+) + e^- \rightarrow AB^+(N_f^+, v_f^+) + e^- \quad (2)$$

various ionized media, occuring in interstellar molecular clouds, supernovae, planetary atmospheres, (plasma assisted) combustion, and atmospheric re-entry of spacecrafts [1]. In this work we use the Multichannel Quantum Defect Theory(MQDT) [2,3] to compute cross sections and rate coefficients of low energy state to state rotational transition for $H_2^+$ . Illustrative result for Inelastic collision (IC) and super elastic collision (SEC) are given and good agreement is obtained with the result of Faure and Tennyson [4]. Cross sections are available for excitation $N_i^+ \longrightarrow N_i^+ + 2$ ($N_i^+ = 0\text{–}8$) and de-excitation $N_i^+ \longrightarrow N_i^+ - 2$ ($N_i^+ = 2\text{–}10$) for electronic energy $10^{-5} \leq \boldsymbol{\varepsilon} \leq 0{,}3$ eV.


## Methodology

To provide updated Inelastic collision(IC) , Super Elastic collision(SEC) cross section and rate coefficients of the benchmark $H_2^+$, we use a step-wise MQDT method. This method treats simultaneously Dissociative Recombination (DR) and related processes and the cross sections of IC and SEC is given by:

$$\sigma^{N,sym}_{N_f^+ v_f^+ \leftarrow N_i^+ v_i^+} = \frac{\pi}{4\varepsilon} \frac{2N+1}{2N_i^+ + 1} \rho^{sym} \sum_{l,l',\Lambda,j} \left| S^{N\Lambda}_{N_f^+ v_f^+ l', N_i^+ v_i^+ l} \right|^2$$

At a given temperature, several $N_i^+$ are accessible for each $v_i^+$

For each set of ' compatible' symmetries of the neutral

a given initial state of ion

$$\sigma_{N_f^+ v_f^+ \leftarrow N_i^+ v_i^+}(V) = \sum_{N,sym} \sigma_{N_f^+ v_f^+ \leftarrow N_i^+ v_i^+}(V)$$

Averaged Boltzman rate coefficients

$$\sigma_{N_f^+ v_f^+ \leftarrow N_i^+ v_i^+}(T) = \left\langle \sigma_{N_f^+ v_f^+ \leftarrow N_i^+ v_i^+}(V) \right\rangle$$

Finally: weighted sum over different symetries

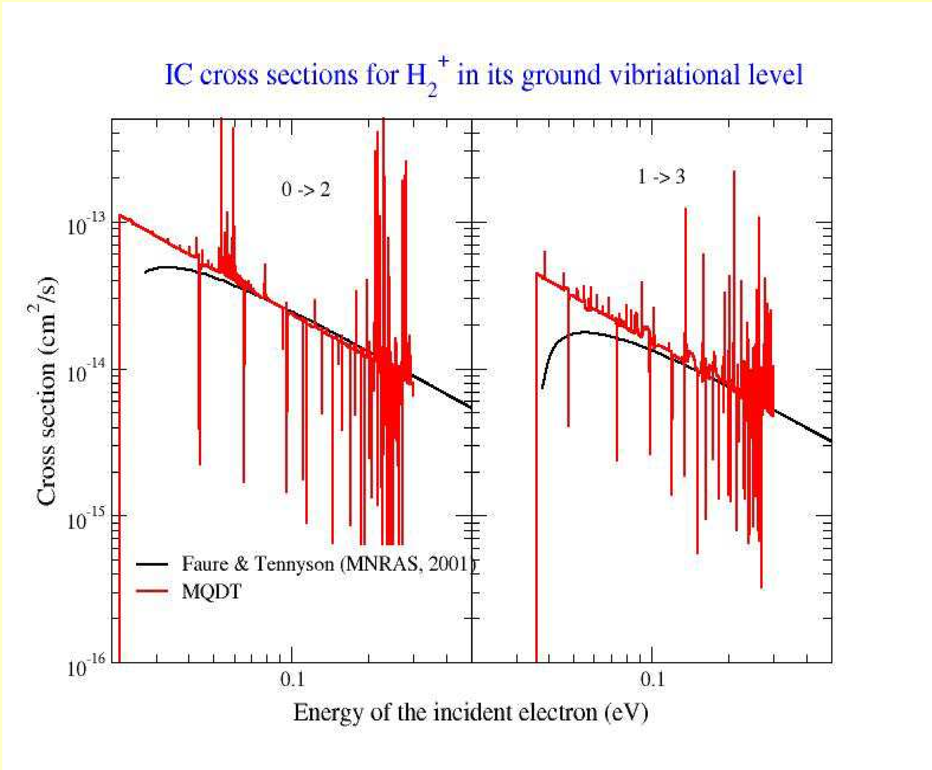
## Motivation

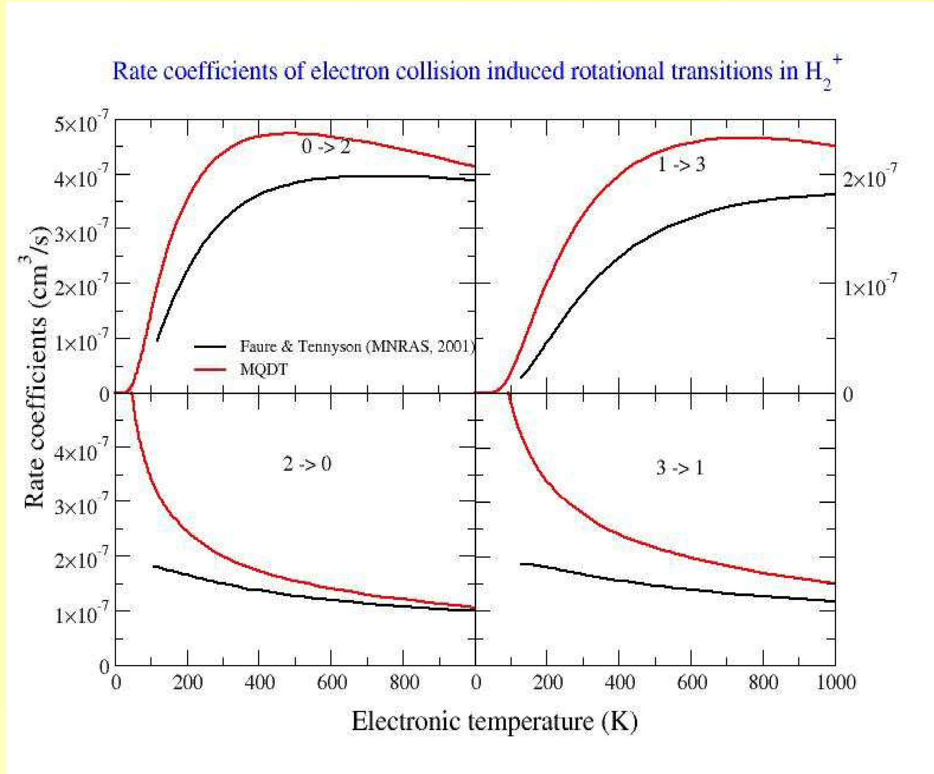
- Perform similar computation than that for $HD^+$ by (Motapon, Argoubi, Pop and al) [5]
- Experimental investigation on the rotational relaxation of $HD^+$ (Shafir and al, Schwalm and al )[6,8]

## Molecular data

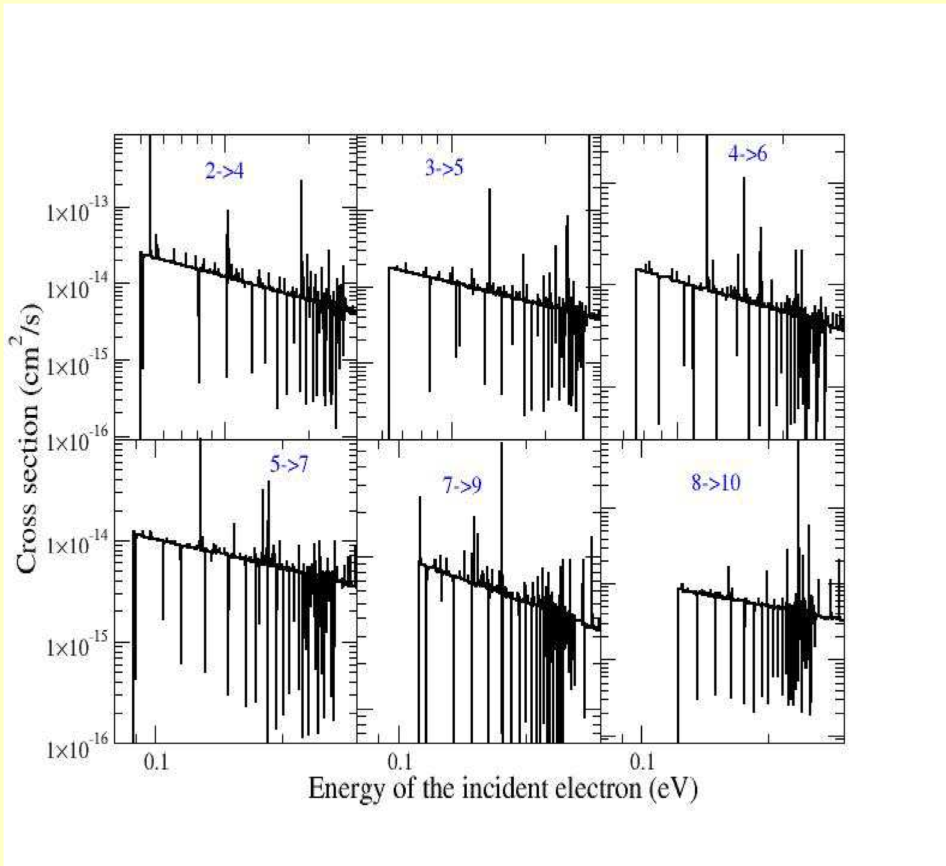
The symmetries included in this work are $^1\Sigma_g^+$, $^1\Pi_g$, $^1\Delta_g$, $^3\Sigma_g^+$, $^3\Pi_g$, $^3\Delta_g$, $^3\Sigma_u^+$ and $^3\Pi_u$ The molecular data (electronic curves and couplings, quantum defect) are those recently used for the $HD^+$ computations. For $^1\Sigma_g^+$ the data are those used by (Motapon and al(2008)[7], Waffeu and al (2011)[8], for the order symmetries new data have been obtained and used in this work.

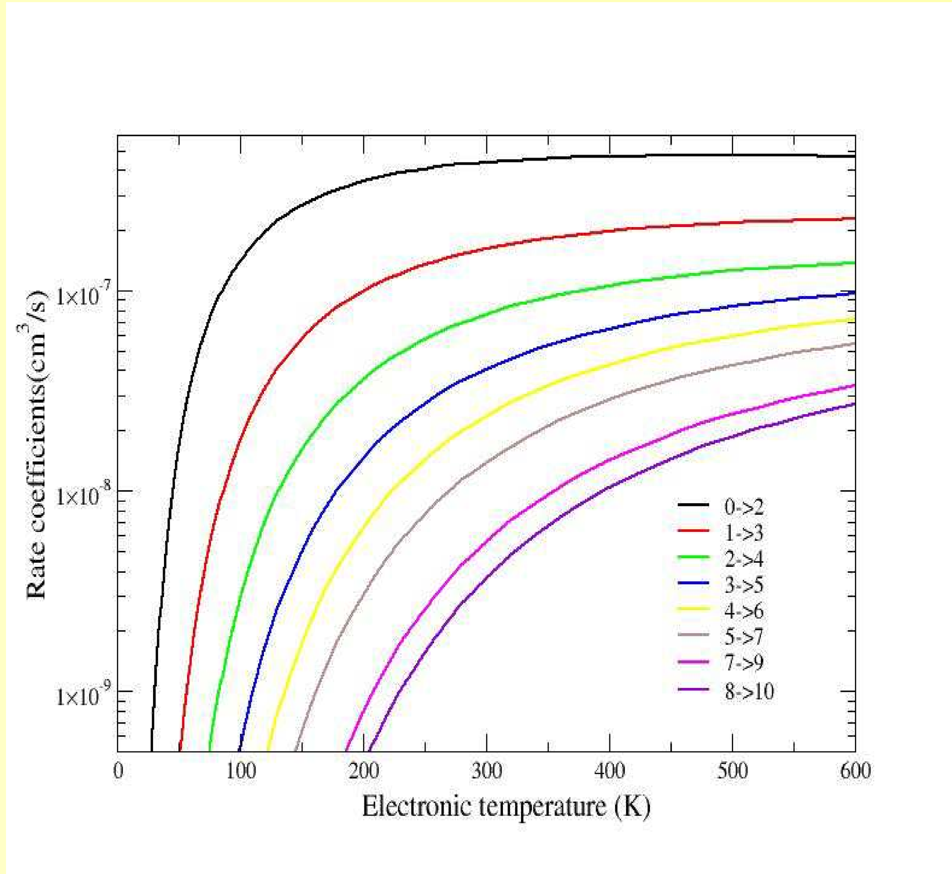
## Comparison for some transitions



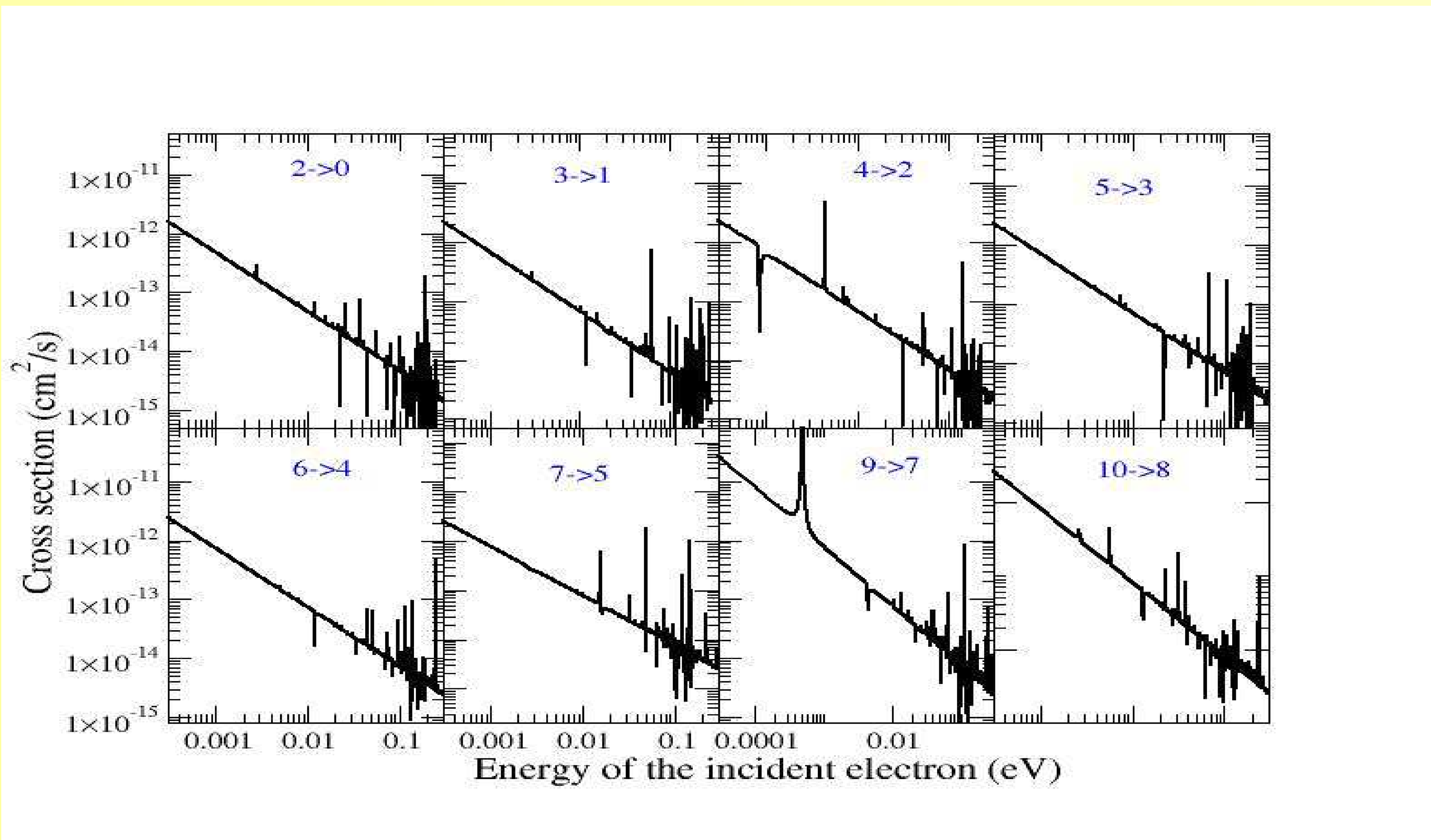



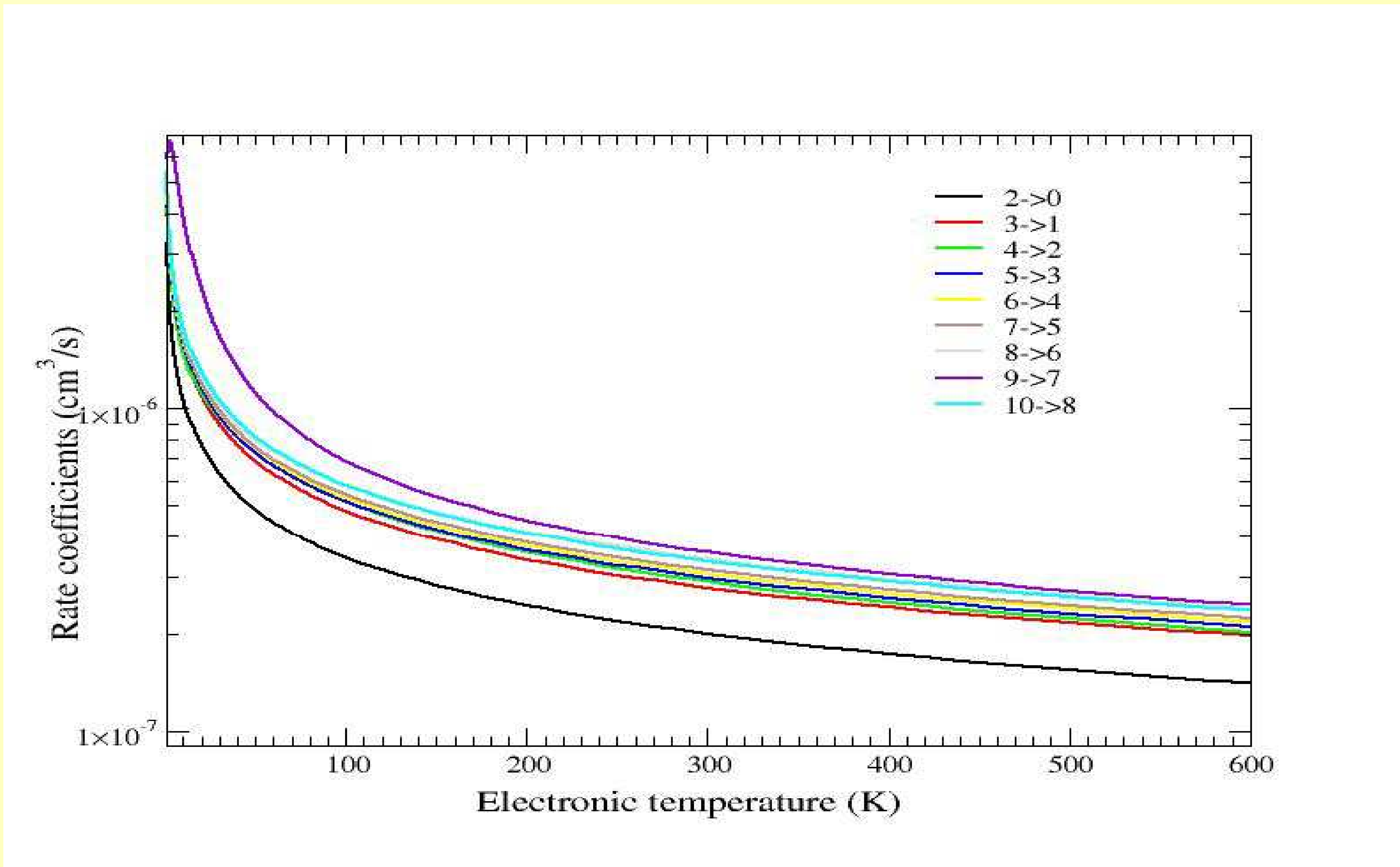

## Cross sections and rate coefficients for Inelastic collisions




## Cross sections and rate coefficients for Super elastic collisions




## Outlook

- The work will be extended to other isotopomers in order to look at isotopic effects
- Participtiion to computations in high energy range (DR and DE) for fusion plasma purpose (collaboration with Kalyan Chakrabarty)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