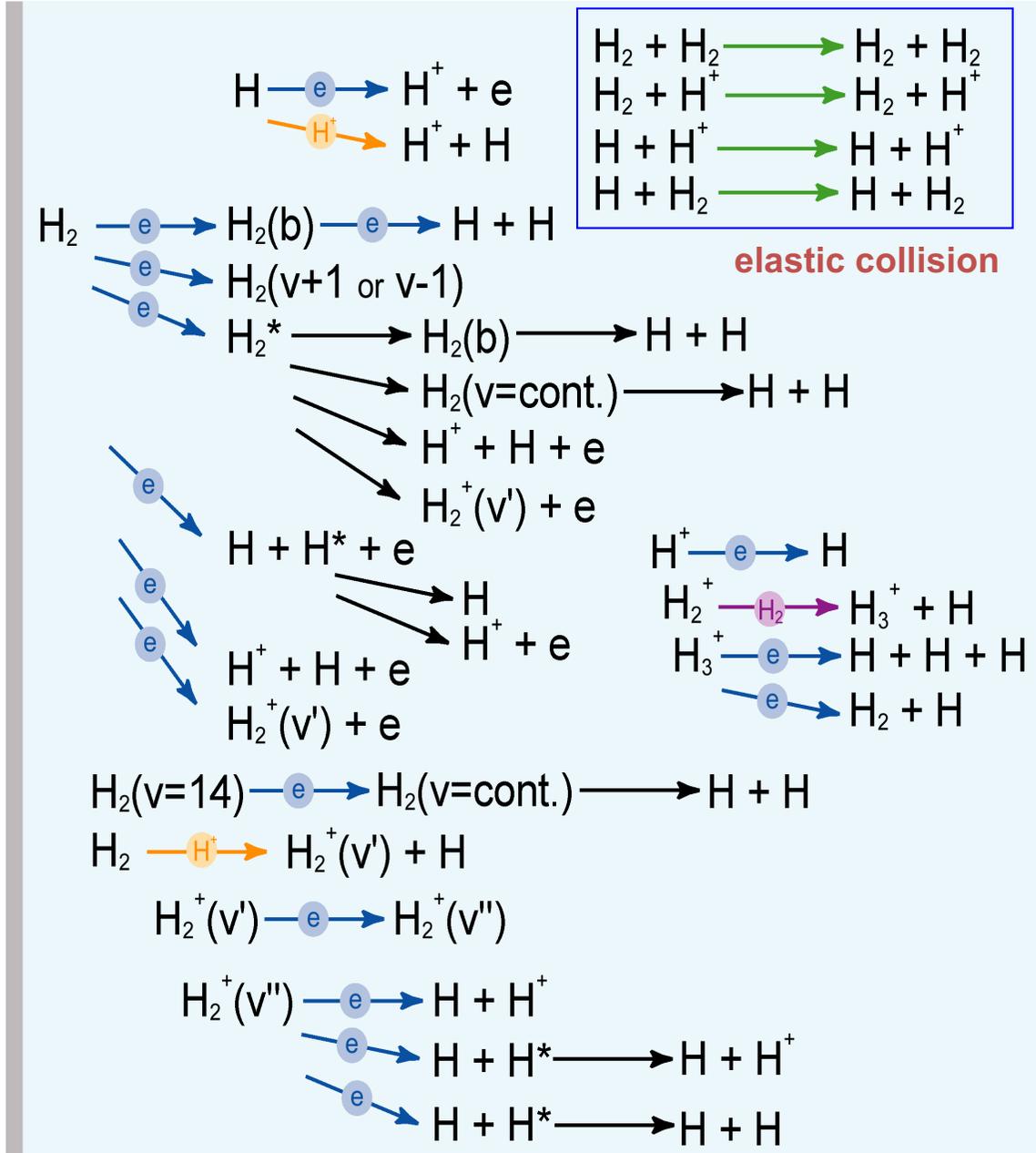


水素分子の電子・振動・回転状態を区別した
衝突輻射モデル・中性粒子輸送コードの構築

澤田圭司

信州大学工学部

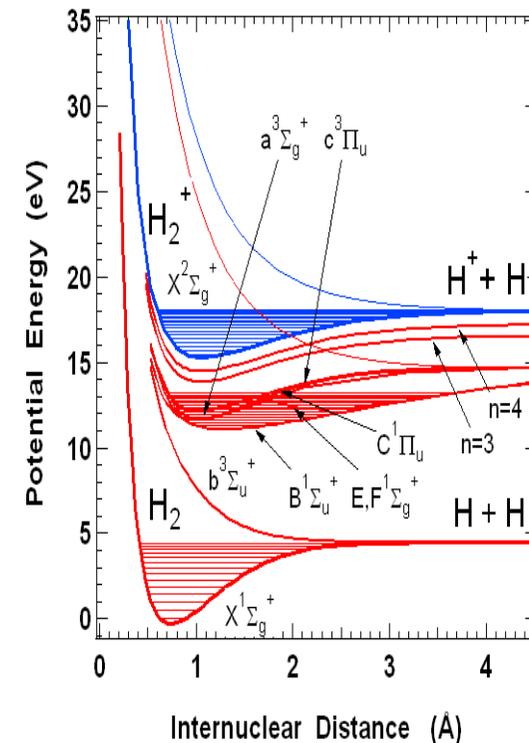
wall



Collisional–Radiative Models

- Hydrogen atom
- Hydrogen molecule (H₂, D₂, HD)
- Helium atom (M. Goto)

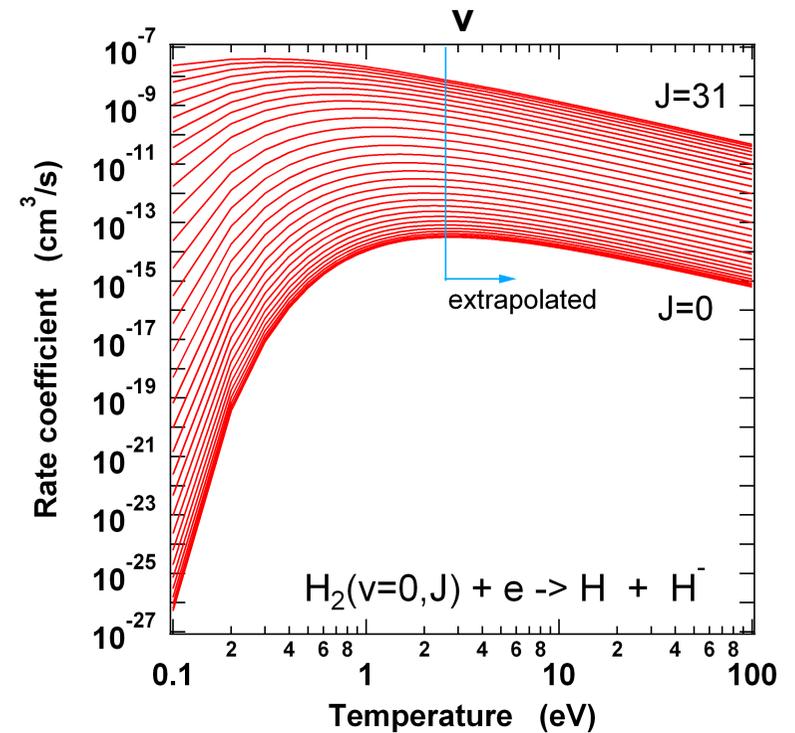
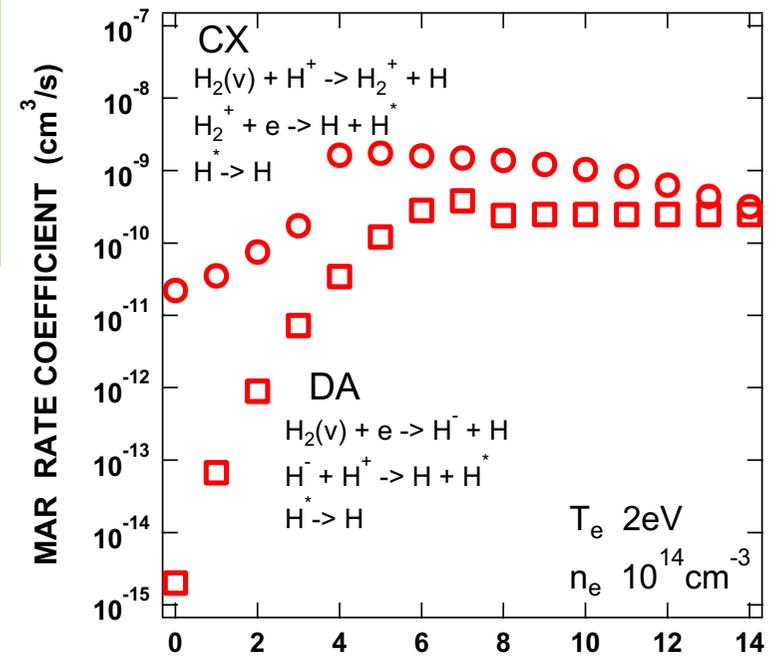
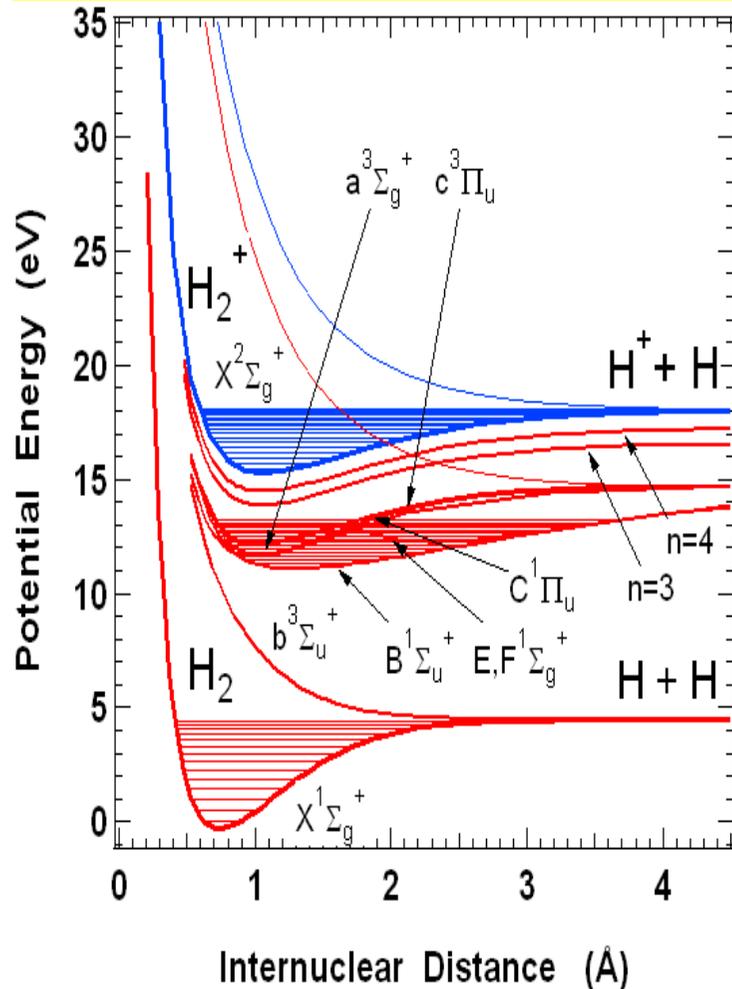
Neutral-Transport Code



H₂ Collisional-Radiative Model

Electronic, vibrational, and rotational states are included.

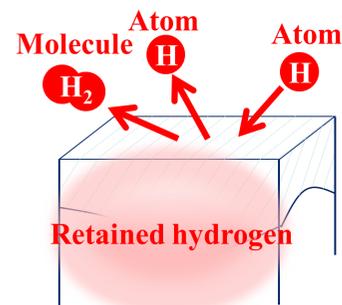
Effective rate coefficients for neutral transport code



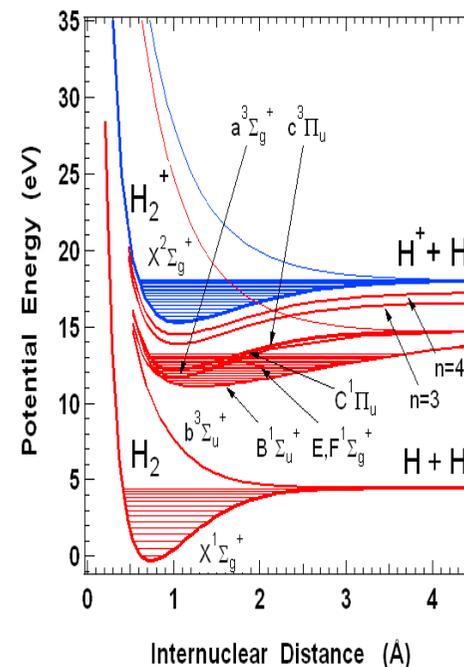
水素分子の電子・振動・回転状態を区別したコードの整備



- (1) ダイバータプラズマの水素分子との衝突によるエネルギー損失の計算 (H₂衝突輻射モデル)
- (2) H₂+H による水素原子のエネルギー損失 (中性粒子輸送コード: 信州大RFプラズマ)
- (3) いろいろな壁材における H の反射・再結合の実験
- (4) HD衝突輻射モデルの構築

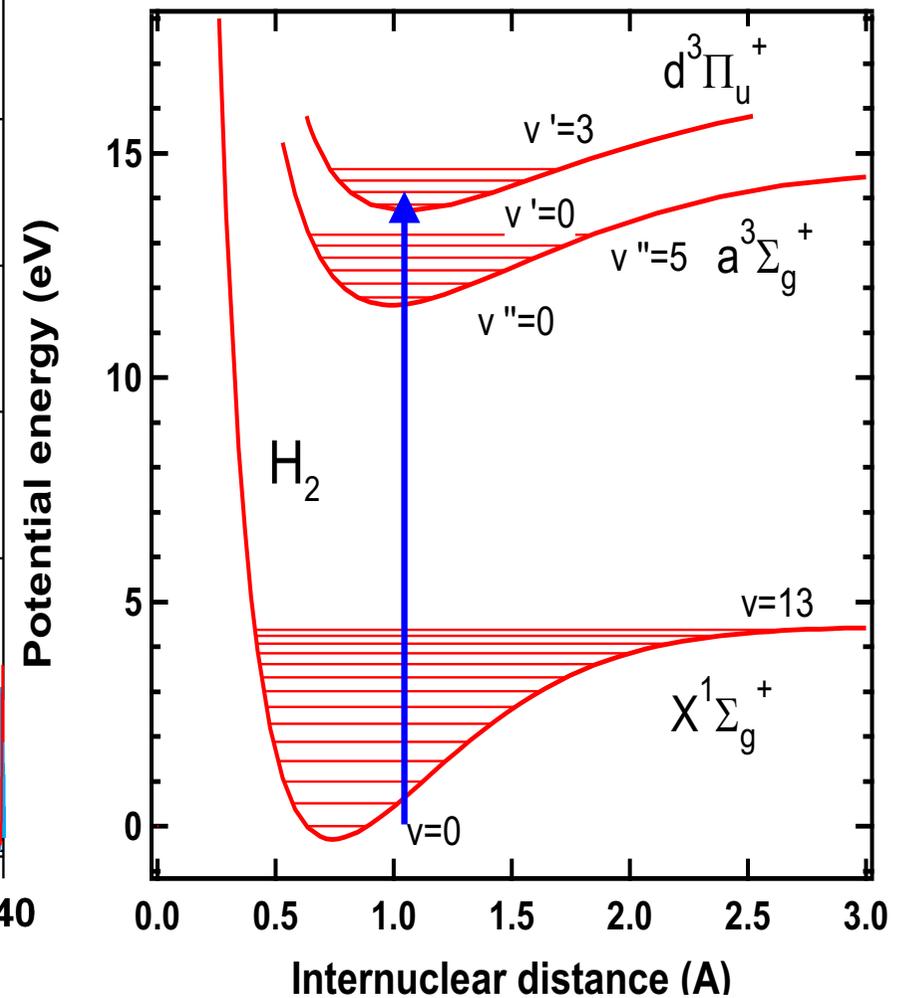
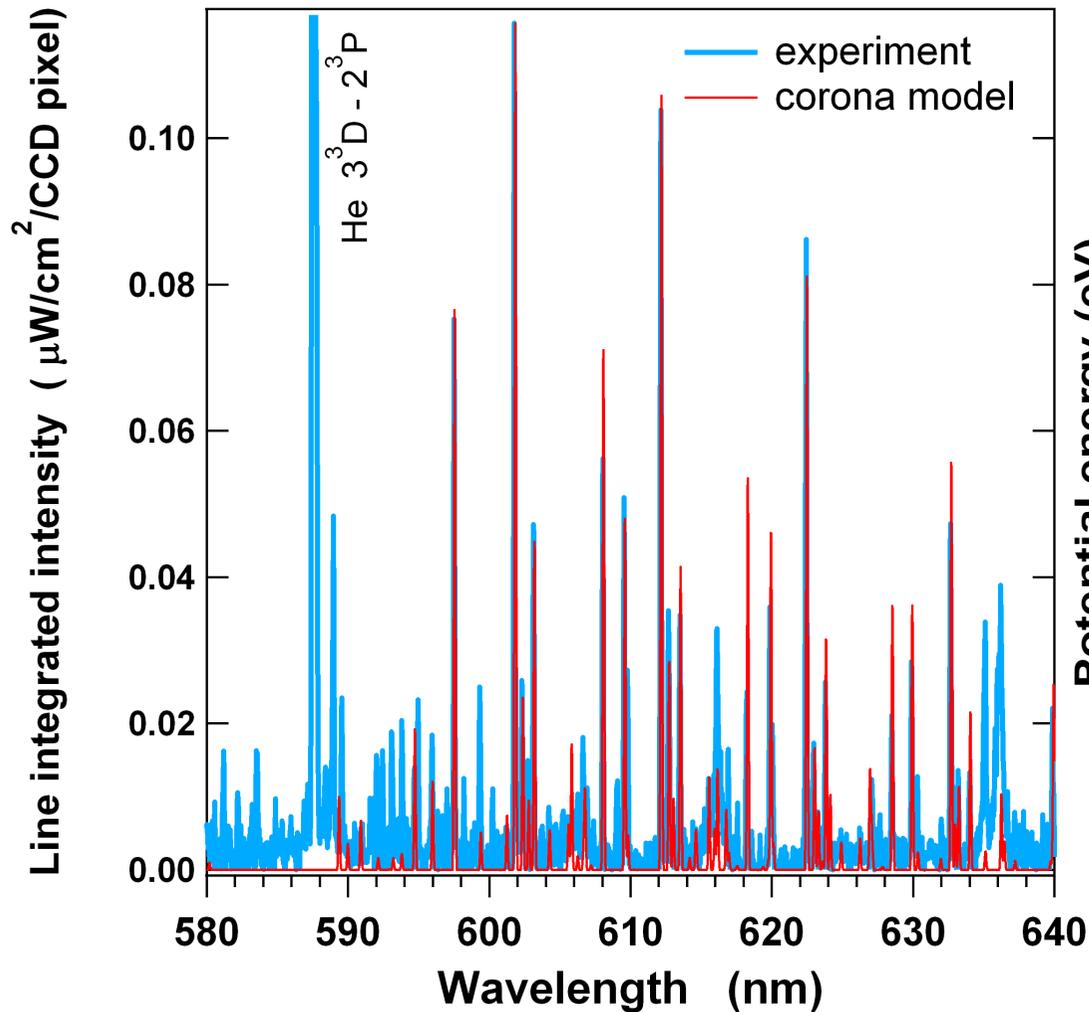
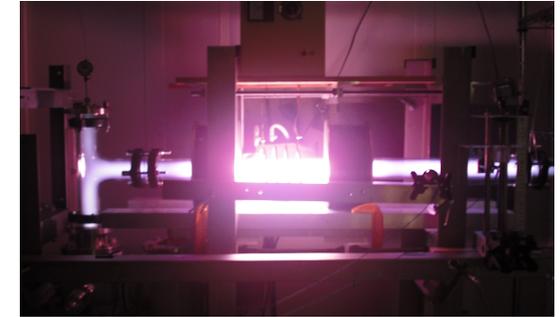


NIFS 中村浩章
 釧路高専 斎藤誠紀

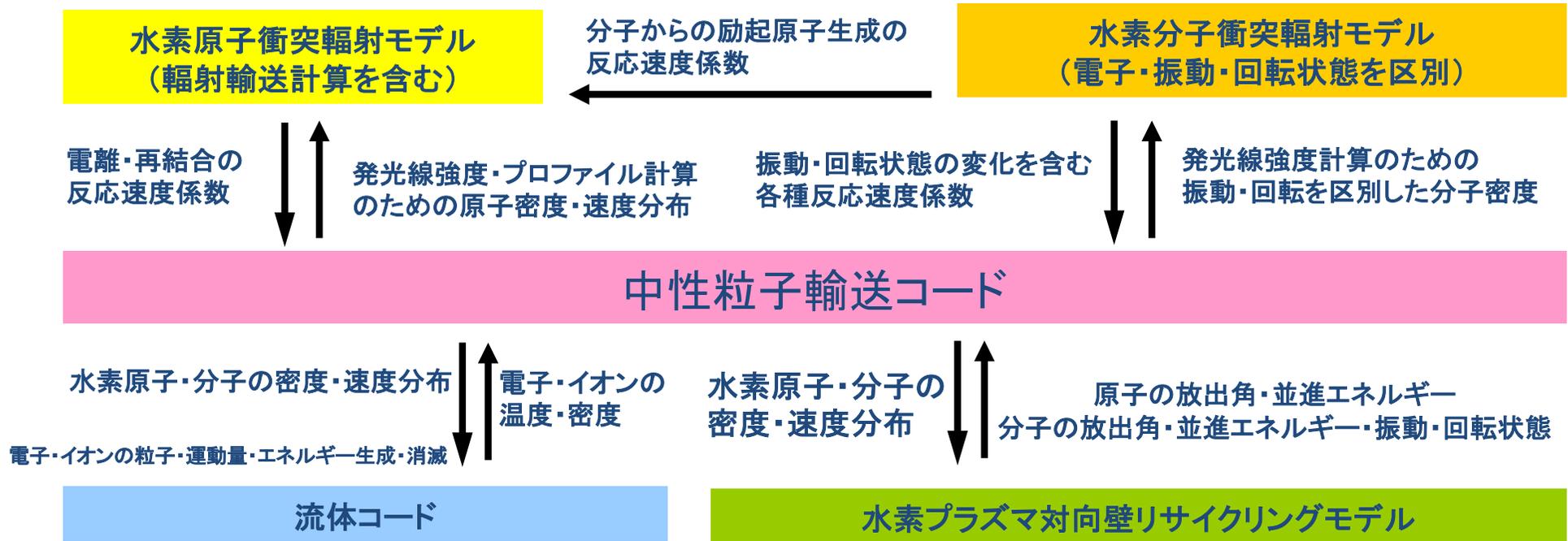


分光計測からの分子の振動・回転ポピュレーション分布の評価

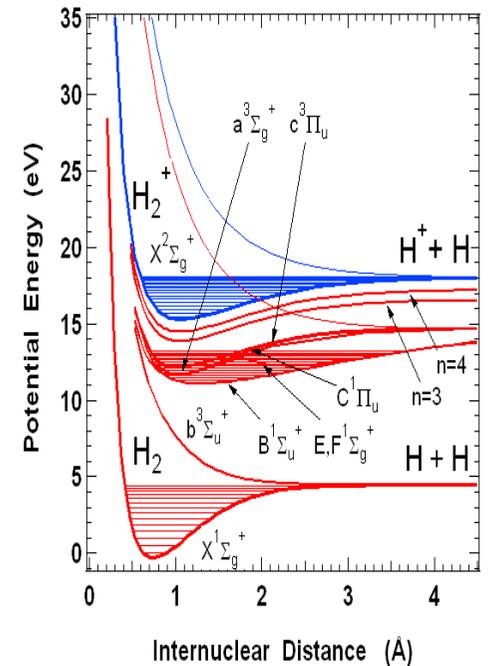
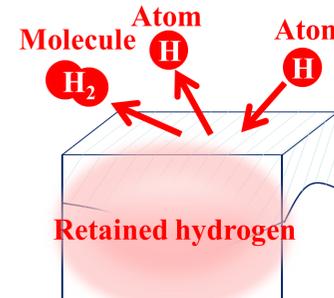
$n_{\text{H}_2} = 7.6 \times 10^{13} \text{ cm}^{-3}$, $T_v = 4200\text{K}$, $T_{\text{rot}} = 350\text{K}$



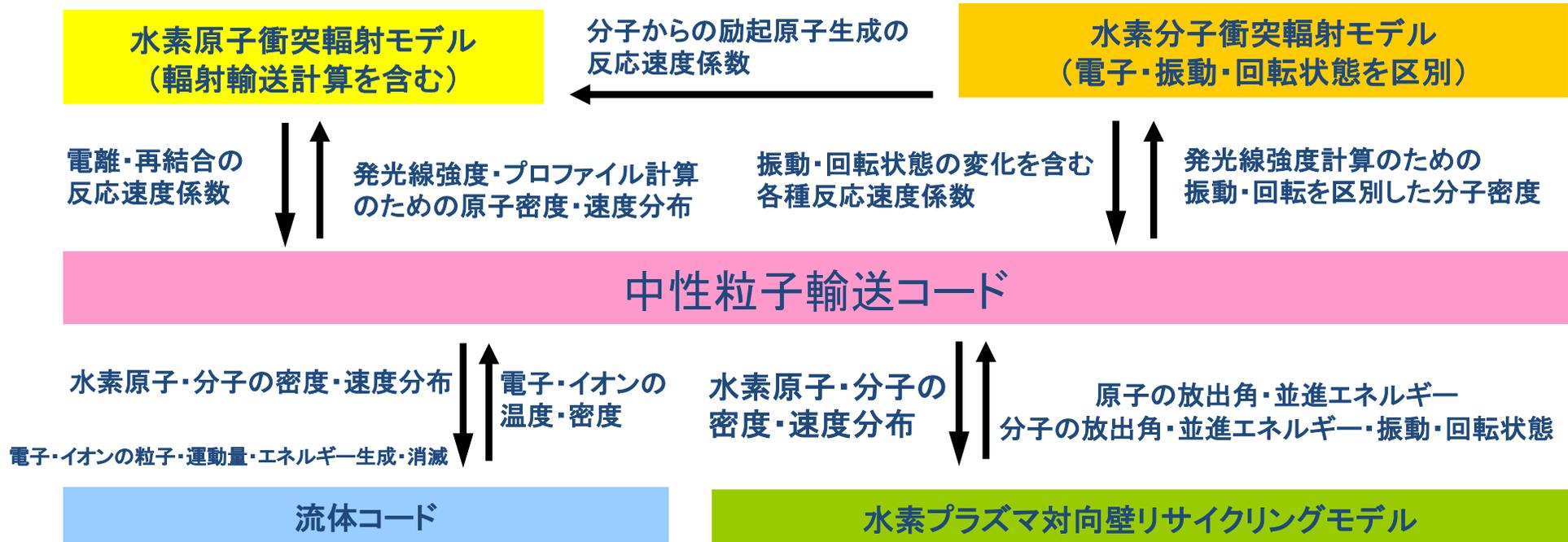
水素分子の電子・振動・回転状態を区別したコードの整備



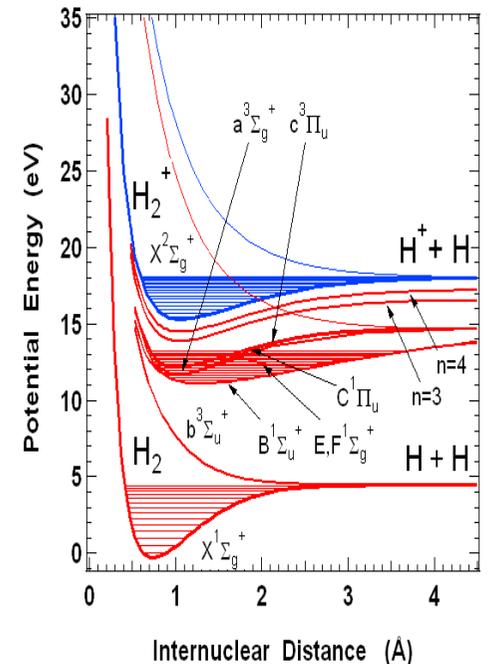
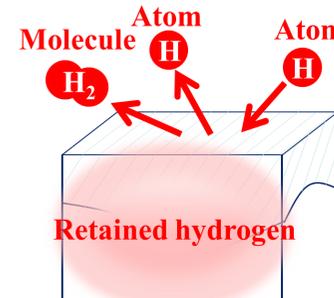
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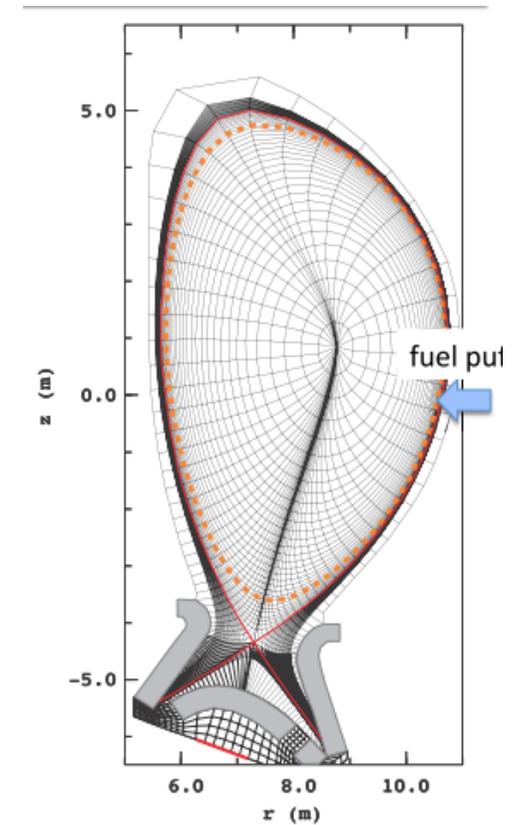
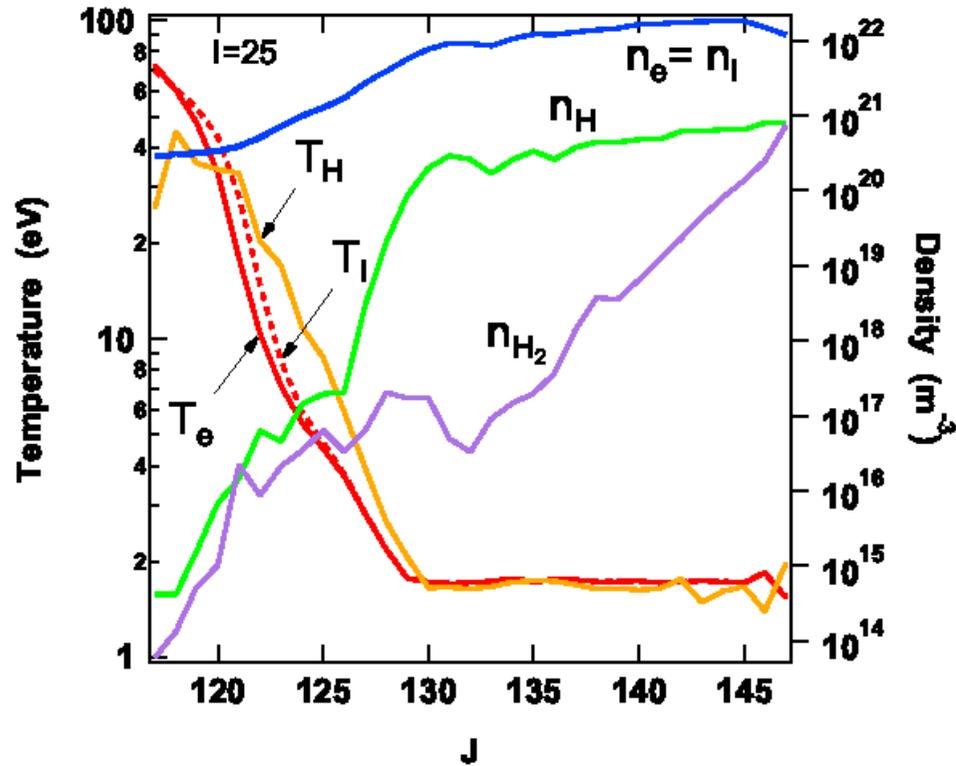
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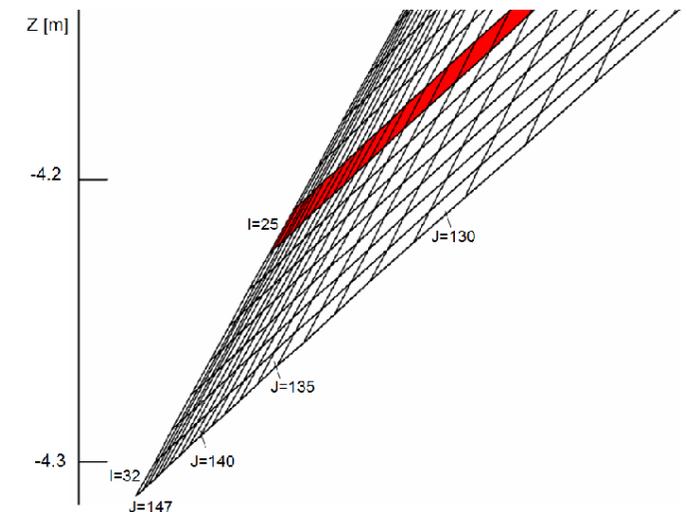


プラズマパラメータ



Plasma $T_e = 2 \text{ eV}$, $T_{H^+} = 2 \text{ eV}$
 $n_e = n_{H^+} = 10^{16} \text{ cm}^{-3}$
 $T_{H_2} = 1 \text{ eV}$, $n_{H_2} = 10^{15} \text{ cm}^{-3}$
 $T_H = 2 \text{ eV}$, $n_H = 10^{15} \text{ cm}^{-3}$

Initial condition 300 K equilibrium



水素分子電子基底状態 振動・回転ポピュレーションの計算



S.A.Wrathmall, D.R. Flower, J. Phys. B 40, 3221-3230 (2007).



J. Horacek et al., Nukleonika 48, 109-112 (2003).

M.A.Morrison and B.C.Saha, Phys. Rev. A 34, 2786-2797 (1986).



A. V. Phelps, J.Phys.Chem. Ref. Data 19, 653-675 (1990).



T.-G.LEE et al., The Astrophysical Journal 689, 1105-1111 (2008).



J. Horacek et al.,

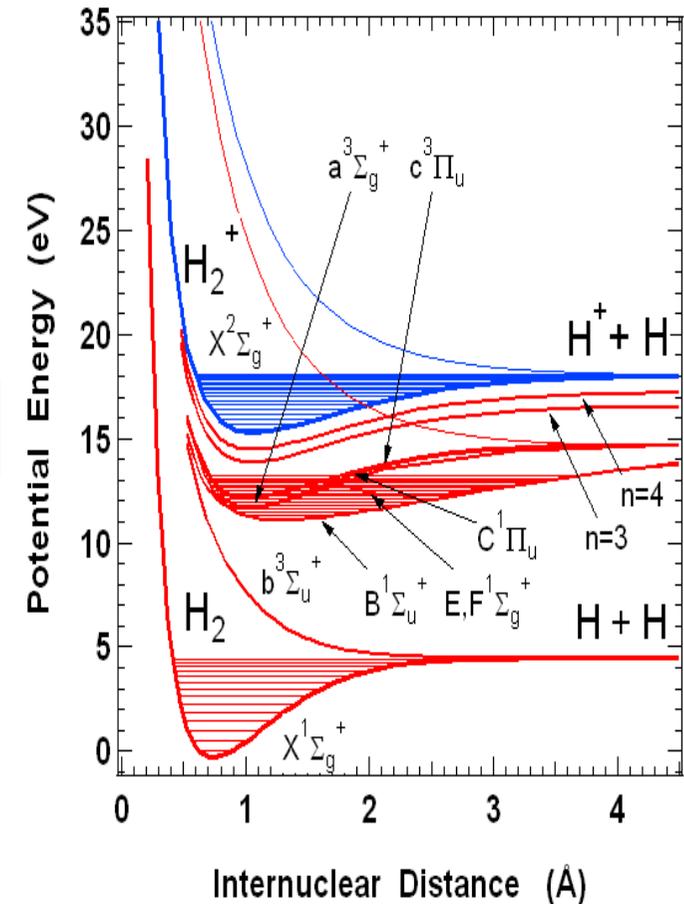
Rate Coefficients for Low-Energy Electron Dissociative Attachment to Molecular Hydrogen, NIFS-DATA-73 (Feb. 2003).



A.Ichihara et al., J. Phys. B 33 4747-4758 (2000).

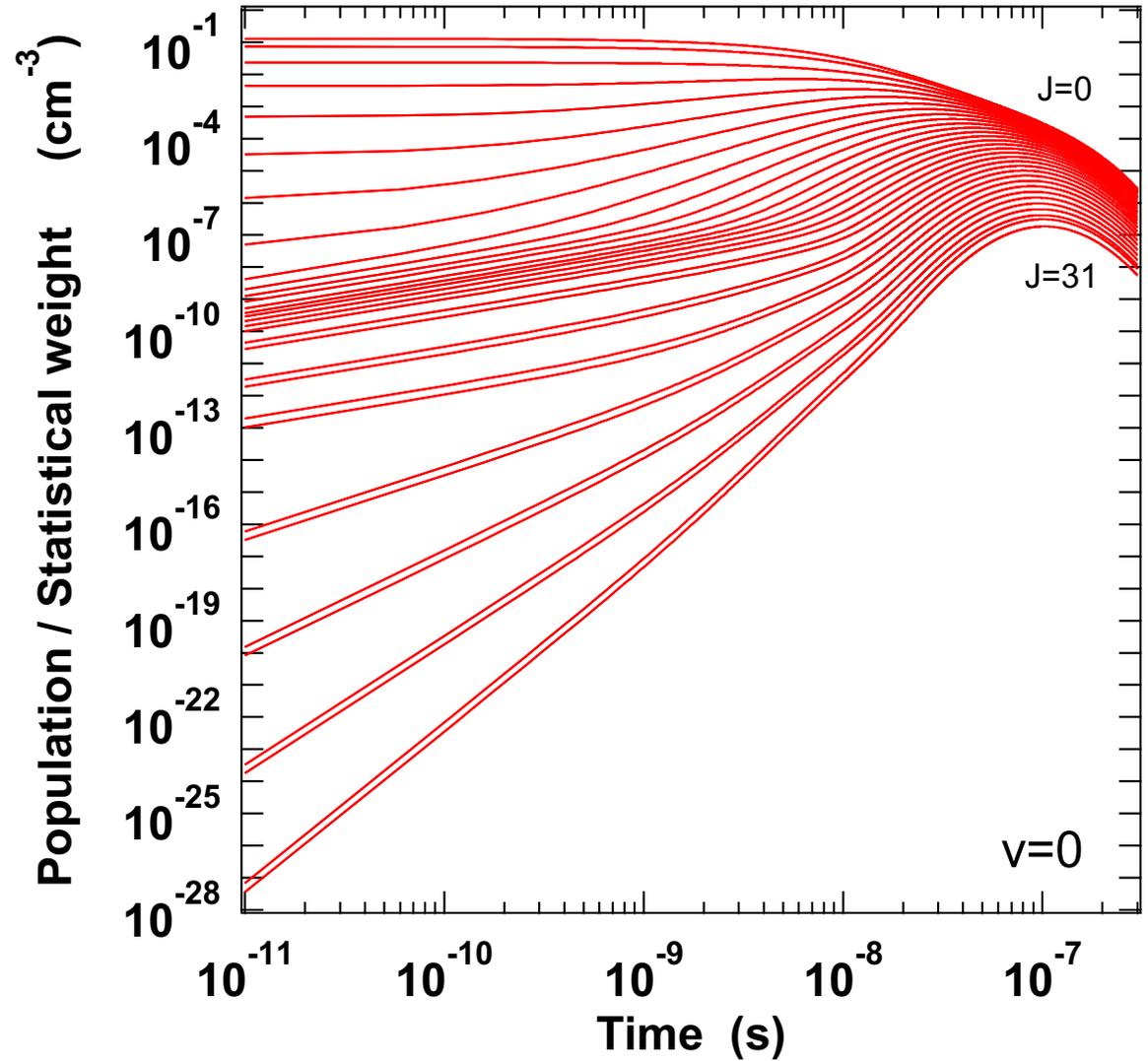
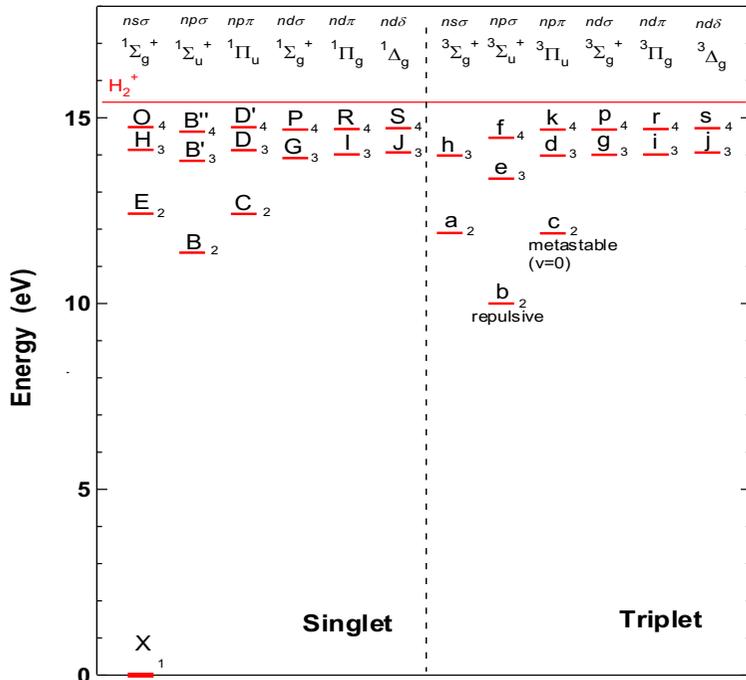
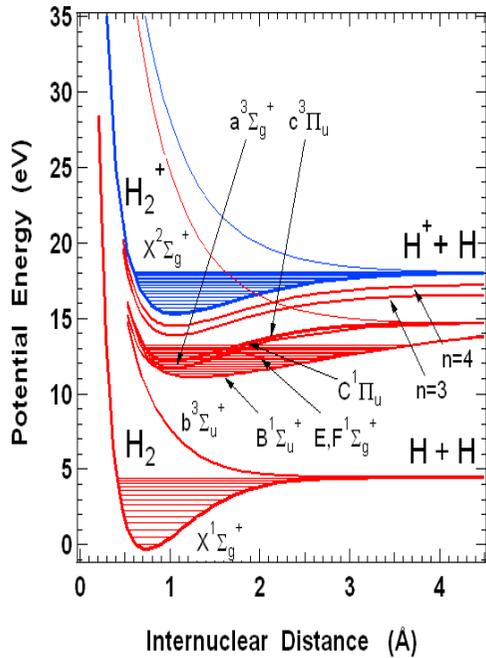


F.Esposito, C.Gorse, M.Capitelli, Chemical Physics Letters 303, 636-640 (1999).



$H_2(X, v=0, J)$

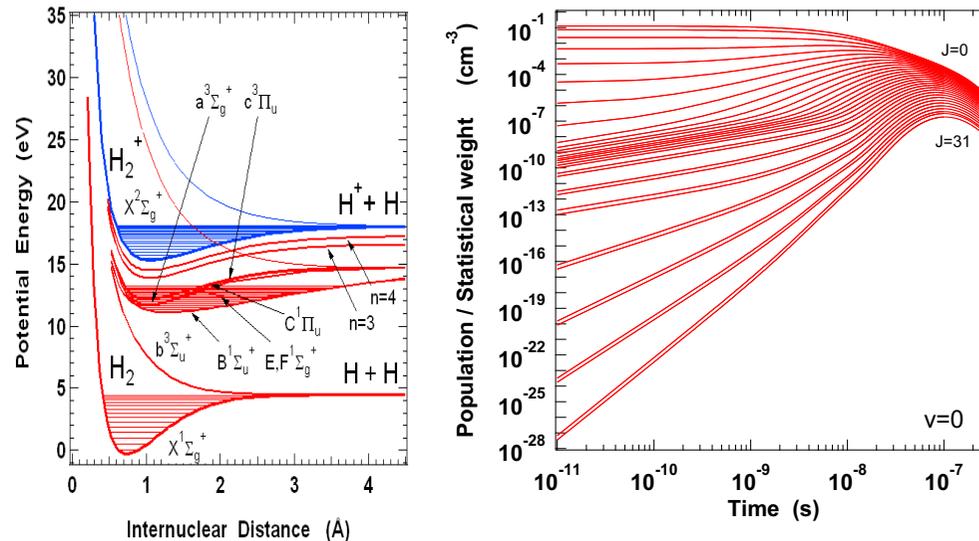
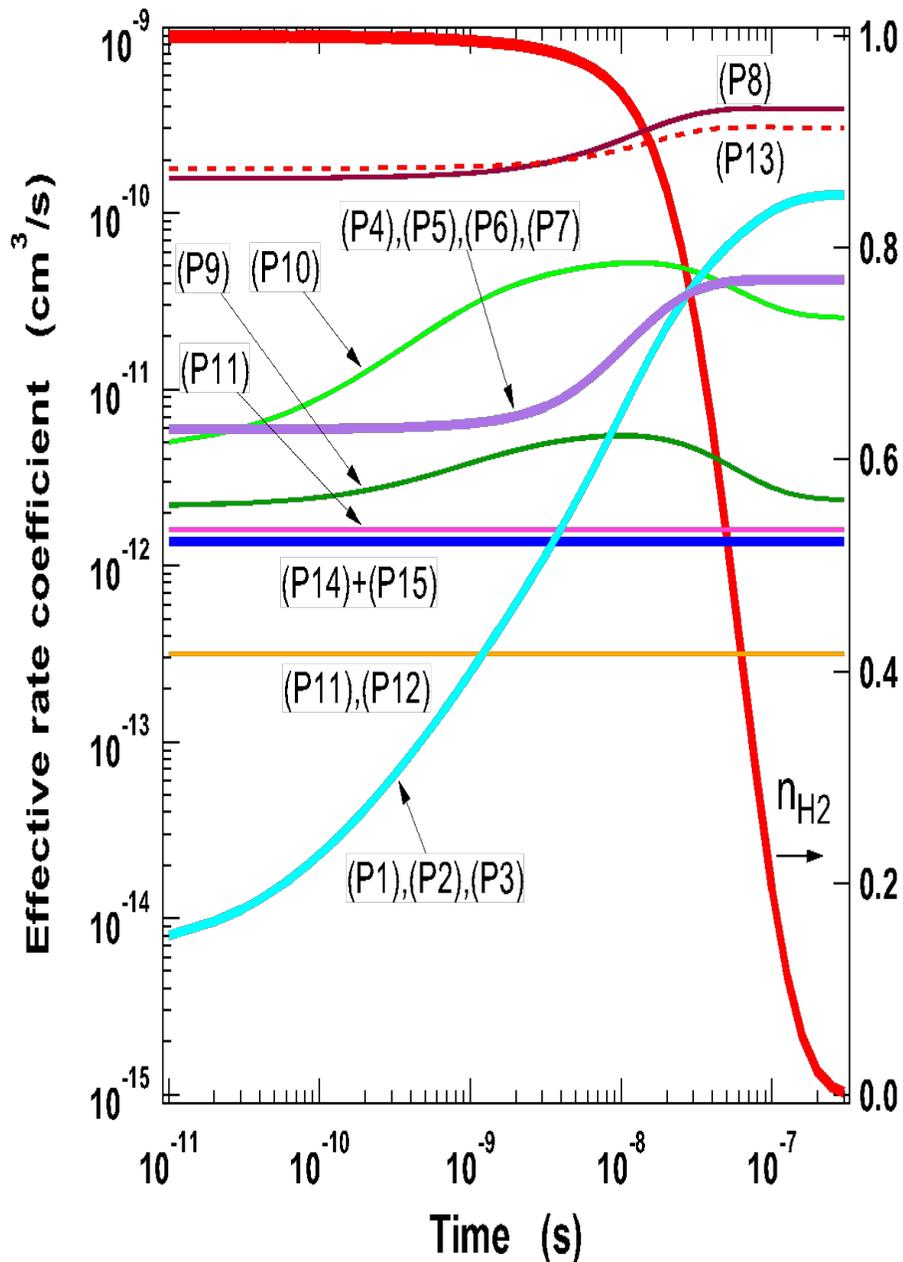
ポピュレーション時間変化



緩和時間

$H_2(X)$ 10^{-9} – 10^{-8} s, $H_2(a)$ 2×10^{-9} s, ほか 10^{-10} s 以下

H₂ 各種反応の速度係数



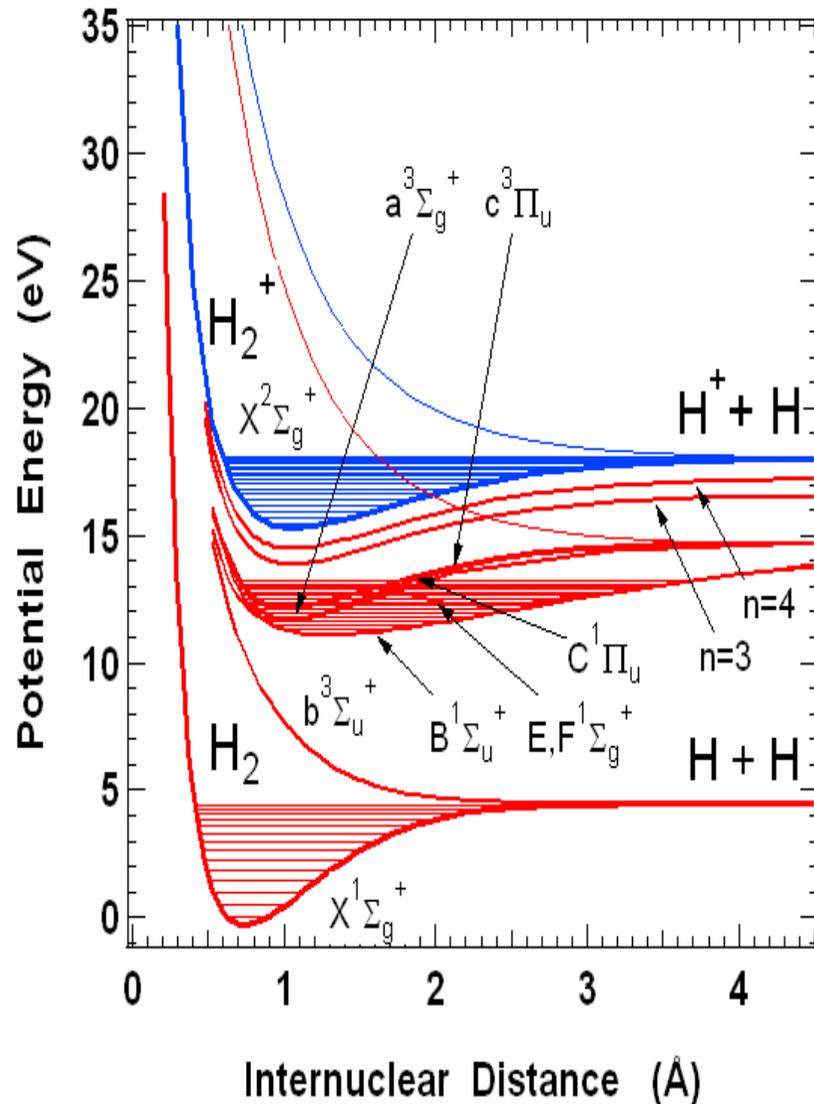
Total H₂ density (cm⁻³)

| Label | Process |
|-------|---|
| (P1) | $\text{H}_2(X^1\Sigma_g^+, v, J) + e \rightarrow \text{H}_2^- \rightarrow \text{H}(p = 1 \text{ or } 2) + \text{H}^-$ |
| (P2) | $\text{H}^- + \text{H}^+ \rightarrow \text{H}(1) + \text{H}(p = 2 \text{ or } 3)$ |
| (P3) | $\text{H}(p = 2 \text{ or } 3) \rightarrow \text{H}^* \rightarrow \text{H}(1)$ |
| (P4) | $\text{H}_2(X^1\Sigma_g^+, v) + \text{H}^+ \rightarrow \text{H}_2^+(X^2\Sigma_g^+, v') \rightarrow \text{H}(1)$ |
| (P5) | $\text{H}_2^+(X^2\Sigma_g^+, v') + e \rightarrow \text{H}_2^+(X^2\Sigma_g^+, v'') + e$ |
| (P6) | $\text{H}_2^+(X^2\Sigma_g^+, v'') + e \rightarrow \text{H}(1) + \text{H}(p \geq 2)$ |
| (P7) | $\text{H}(p \geq 2) \rightarrow \text{H}^* \rightarrow \text{H}(1)$ |
| (P8) | $\text{H}_2(X^1\Sigma_g^+, v) + e \rightarrow \text{H}_2(b^3\Sigma_u^+) + e \rightarrow \text{H}(1) + \text{H}(1)$ |
| (P9) | $\text{H}_2^*(\text{singlet}, v, J) \rightarrow \text{H}_2(X^1\Sigma_g^+) + h\nu \rightarrow \text{H}(1) + \text{H}(1)$ |
| (P10) | $\text{H}_2^*(\text{triplet}, v, J) \rightarrow \text{H}_2(b^3\Sigma_u^+) + h\nu \rightarrow \text{H}(1) + \text{H}(1)$ |
| (P11) | $\text{H}_2(X^1\Sigma_g^+) + e \rightarrow \text{H}(1) + \text{H}(p \geq 2)$ |
| (P12) | $\text{H}(p \geq 2) \rightarrow \text{H}^* \rightarrow \text{H}(1)$ |
| (P13) | $\text{H}_2(X^1\Sigma_g^+, v) + \text{H} \rightarrow \text{H} + \text{H} + \text{H}$ |
| (P14) | $\text{H}^+ + e \rightarrow \text{H}(1)$ |
| (P15) | $\text{H}^+ + e \rightarrow \text{H}^* \rightarrow \text{H}(1)$ |
| (P16) | $\text{H}_2^+(X^2\Sigma_g^+, v') + e \rightarrow \text{H}(1) + \text{H}^+ + e$ |
| (P17) | $\text{H}_2^+ + \text{H}_2 \rightarrow \text{H}_3^+ + \text{H}$ |
| (P18) | $\text{H}_3^+ + e \rightarrow \text{H}_2(X^1\Sigma_g^+, v, J) + \text{H} \text{ or } \text{H} + \text{H} + \text{H}$ |

H₂ 各種反応の速度係数

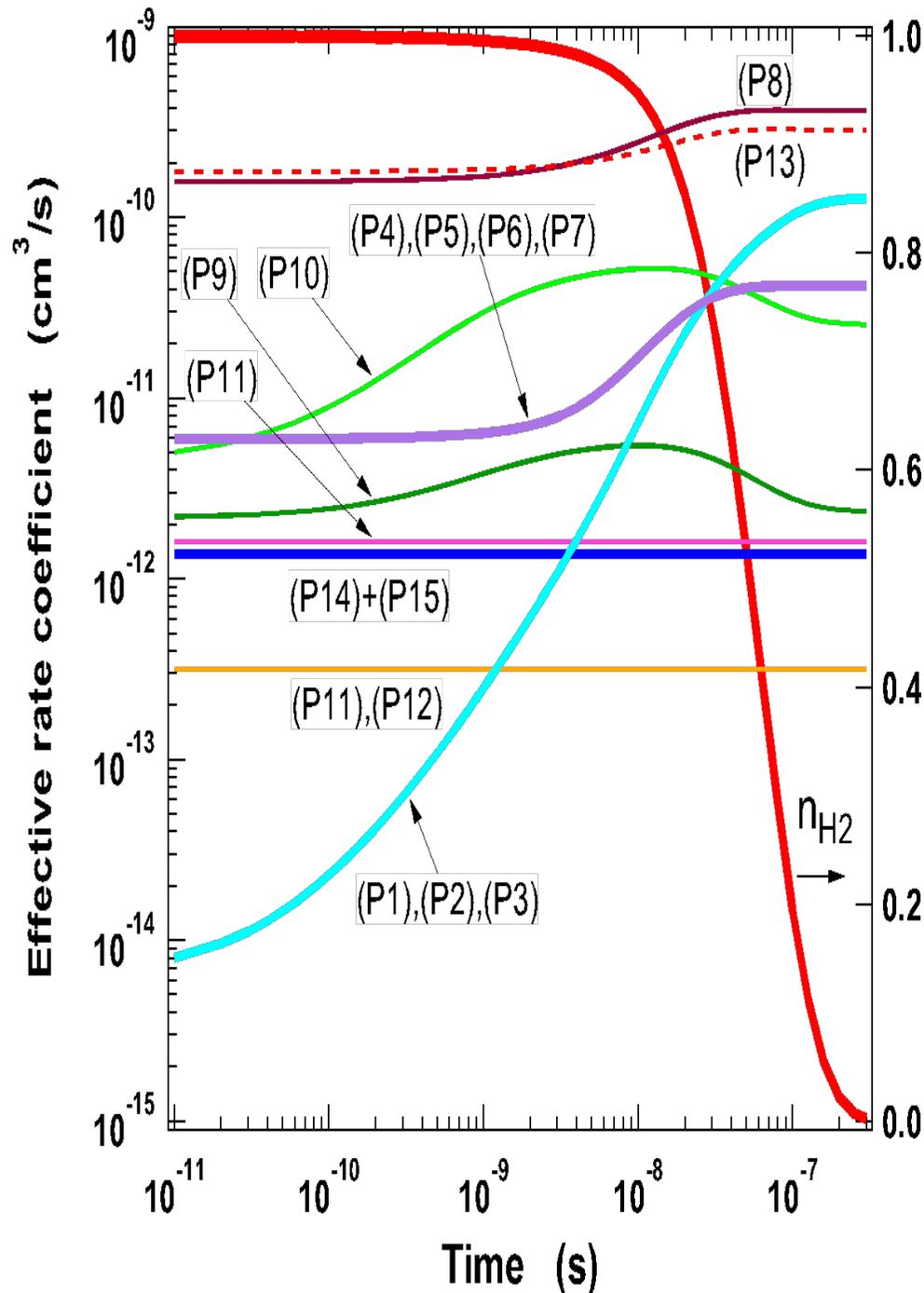
$$\frac{dn_{\text{H}}}{dt} = P_{\text{H}_2}^{\text{H}} n_{\text{H}_2} n_e$$

$$\frac{dn_{\text{H}}}{dt} = P_{\text{H}^+}^{\text{H}} n_{\text{H}^+} n_e$$

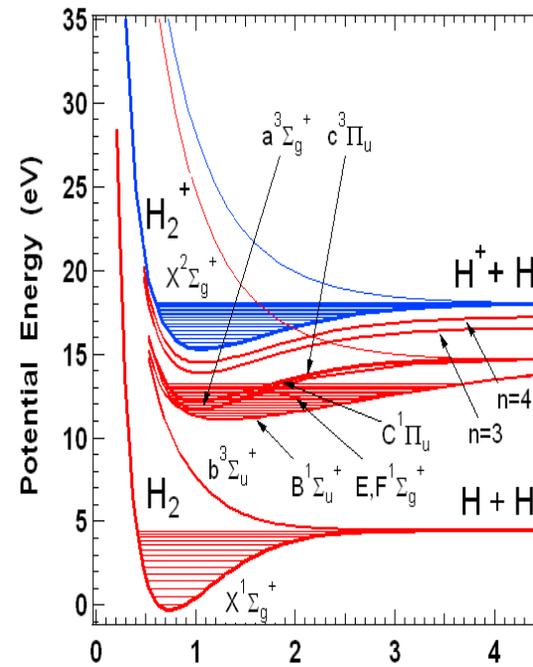


| Label | Process |
|-------|---|
| (P1) | $\text{H}_2(X^1\Sigma_g^+, v, J) + e \rightarrow \text{H}_2^- \rightarrow \text{H}(p = 1 \text{ or } 2) + \text{H}^-$ |
| (P2) | $\text{H}^- + \text{H}^+ \rightarrow \text{H}(1) + \text{H}(p = 2 \text{ or } 3)$ |
| (P3) | $\text{H}(p = 2 \text{ or } 3) \rightarrow \text{H}^* \rightarrow \text{H}(1)$ |
| (P4) | $\text{H}_2(X^1\Sigma_g^+, v) + \text{H}^+ \rightarrow \text{H}_2^+(X^2\Sigma_g^+, v') \rightarrow \text{H}(1)$ |
| (P5) | $\text{H}_2^+(X^2\Sigma_g^+, v') + e \rightarrow \text{H}_2^+(X^2\Sigma_g^+, v'') + e$ |
| (P6) | $\text{H}_2^+(X^2\Sigma_g^+, v'') + e \rightarrow \text{H}(1) + \text{H}(p \geq 2)$ |
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H₂ 各種反応の速度係数

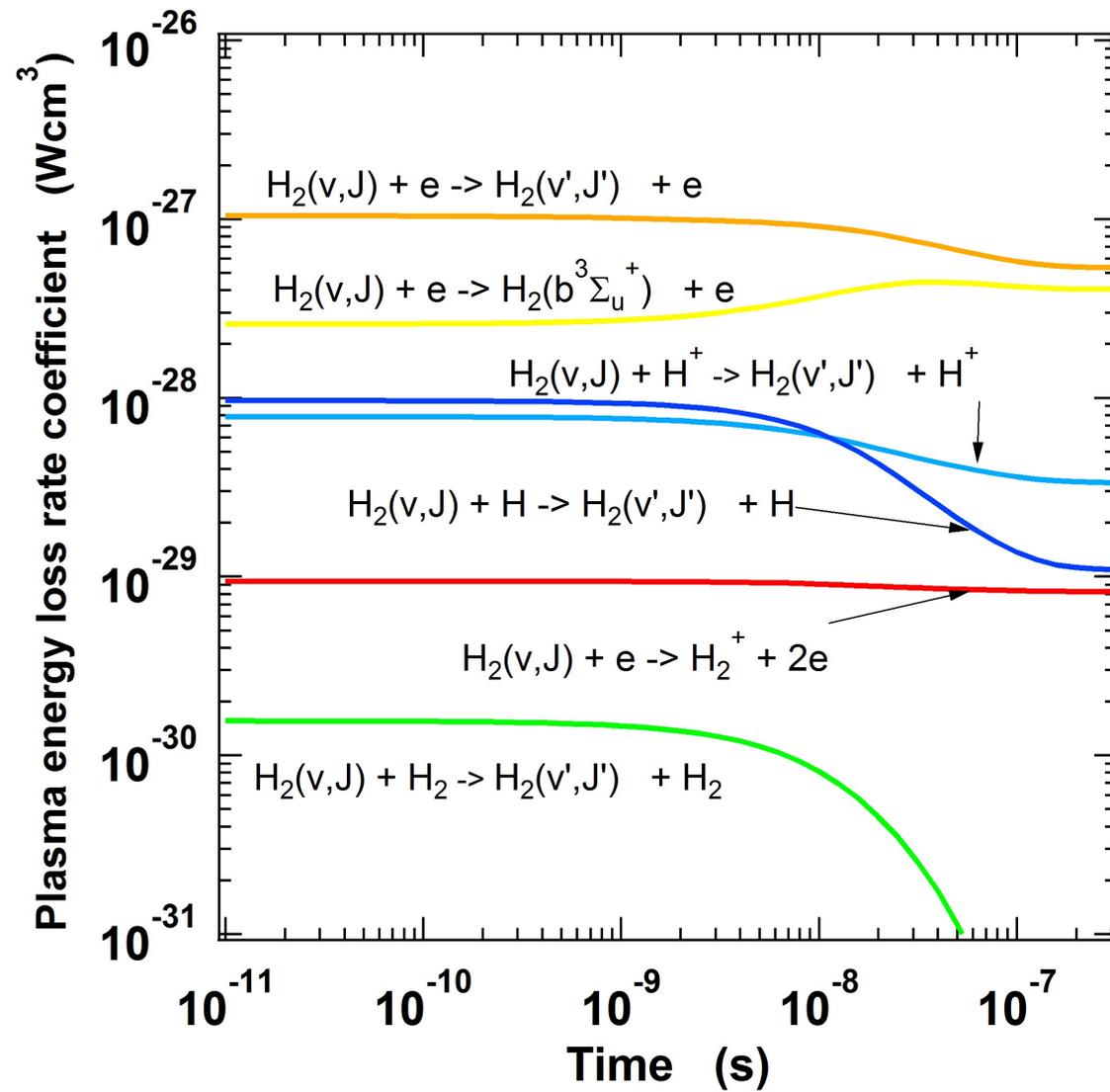
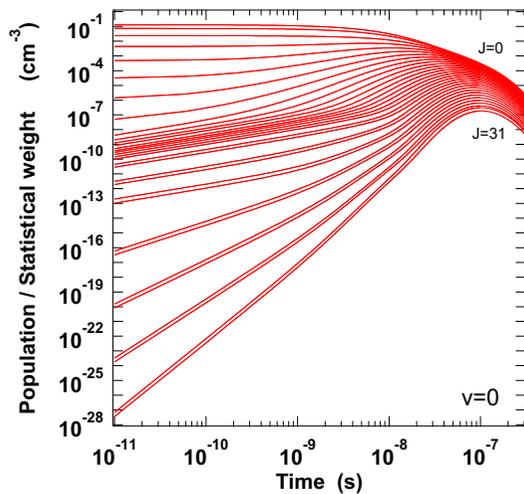
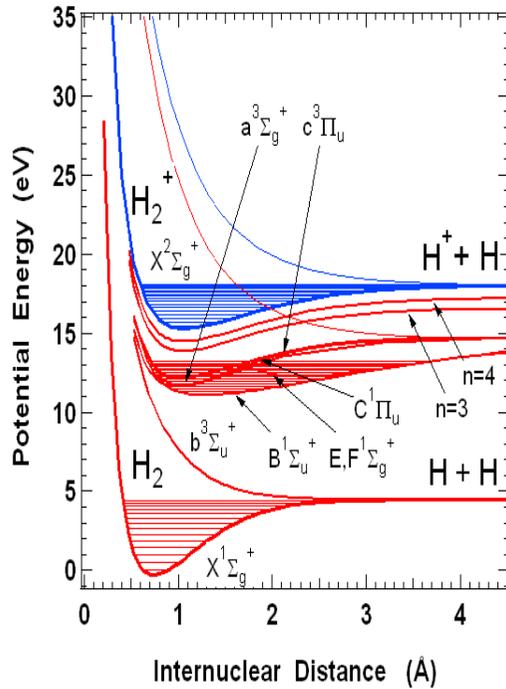


Total H₂ density (cm⁻³)



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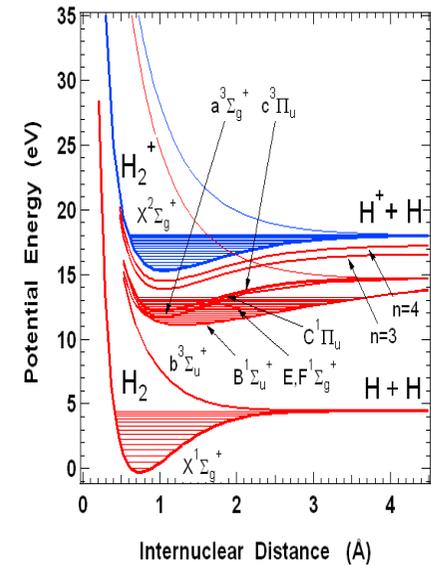
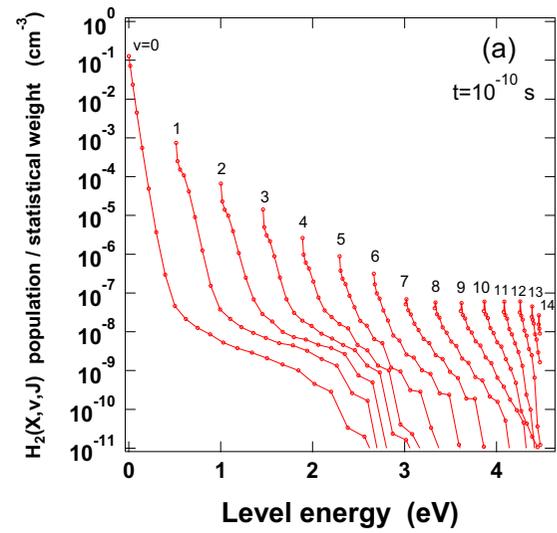
H₂ との衝突による プラズマ粒子の エネルギー損失



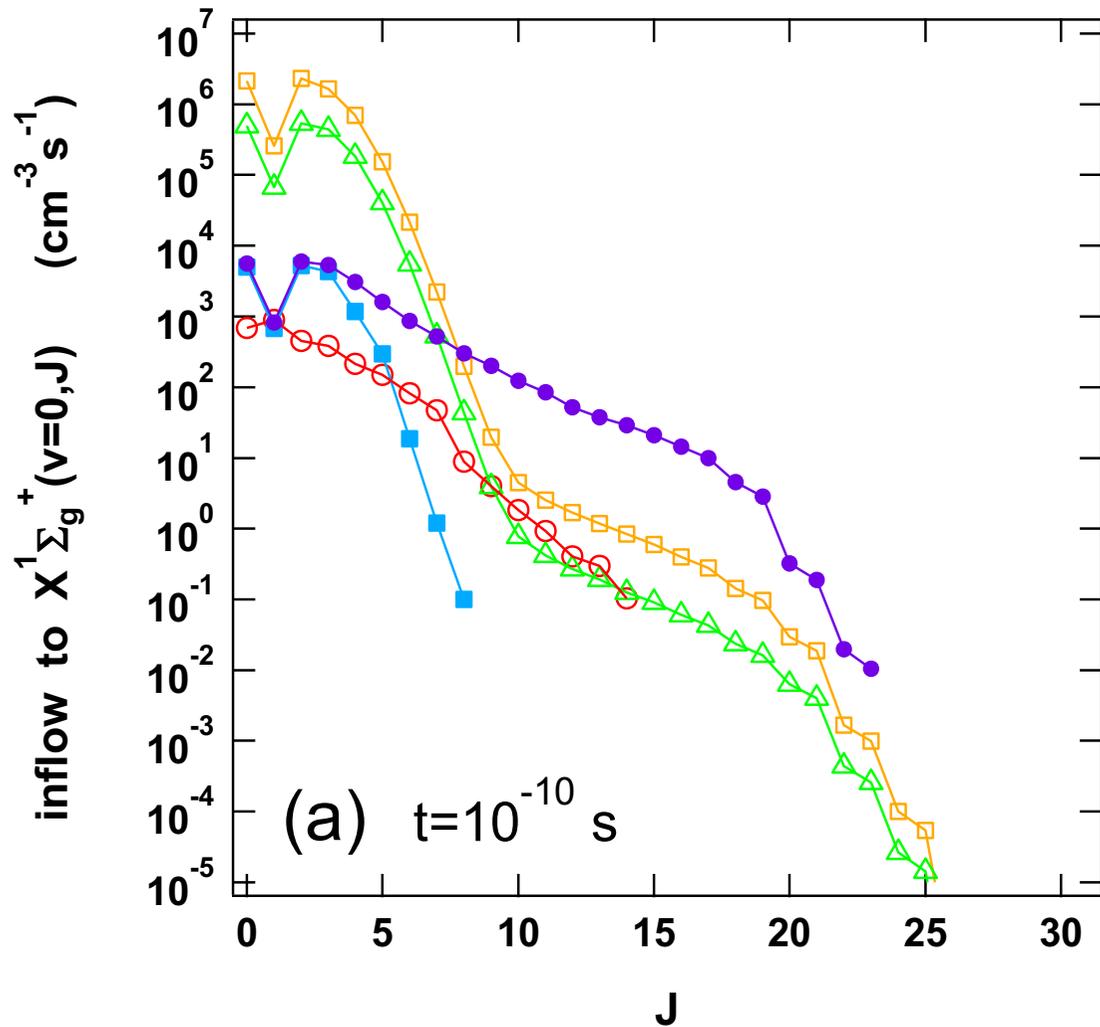
$T_e = 2 \text{ eV}, T_{H^+} = 2 \text{ eV}$
 $n_e = n_{H^+} = 10^{16} \text{ cm}^{-3}$
 $T_{H_2} = 1 \text{ eV}, n_{H_2} = 10^{15} \text{ cm}^{-3}$
 $T_H = 2 \text{ eV}, n_H = 10^{15} \text{ cm}^{-3}$

H₂(X, v, J) ポピュレーション 流入・流出 (10⁻¹⁰ sec)

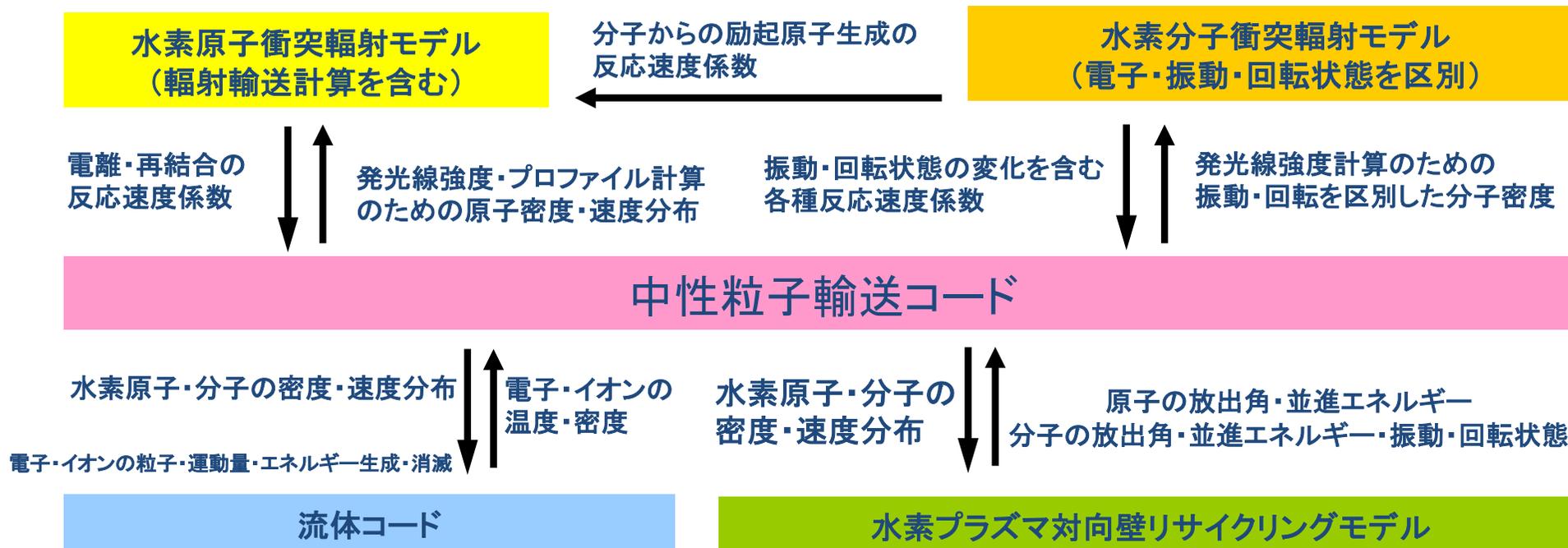
- (open circle) emission from the electronic excited states
- (open square) electron collision transition in X
- (triangle) proton collision transition in X
- (closed circle) atomic collision transition in X
- (closed square) molecular collision transition in X



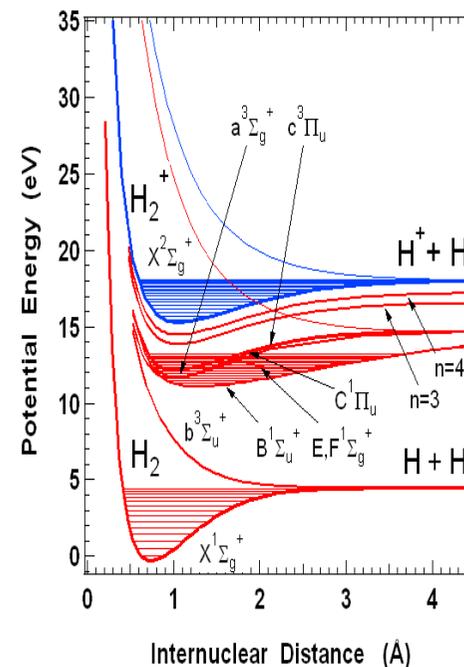
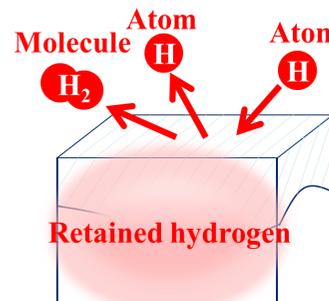
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水素分子の電子・振動・回転状態を区別したコードの整備



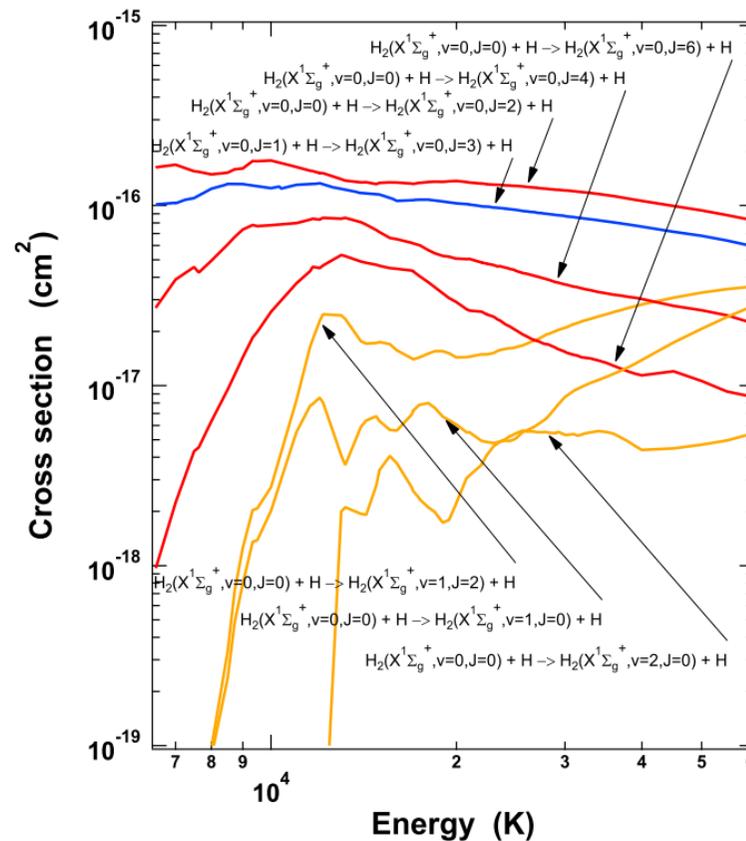
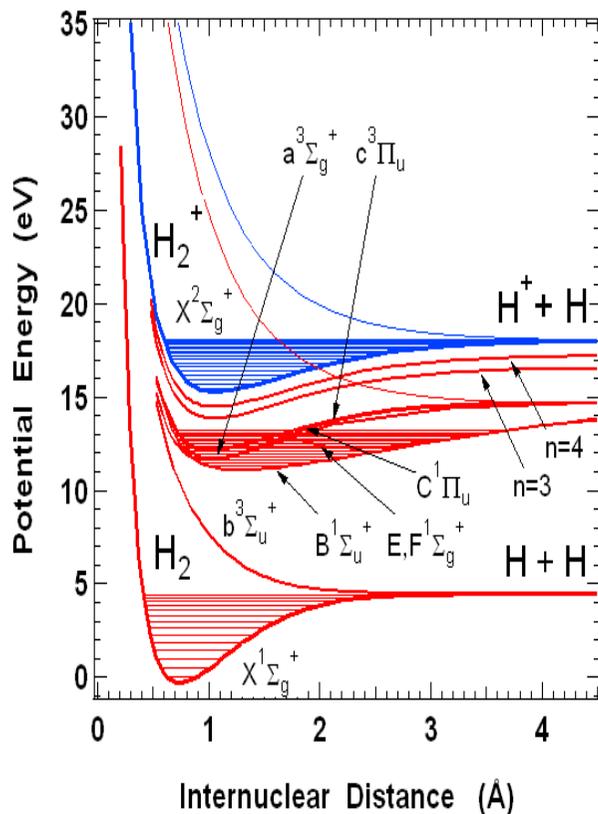
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- (3) いろいろな壁材における H の反射・再結合の実験
- (4) HD衝突輻射モデルの構築



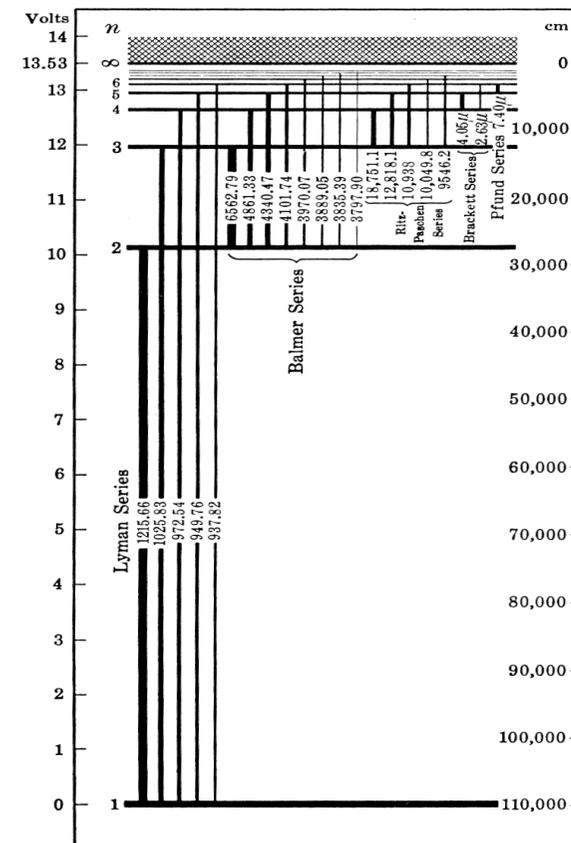
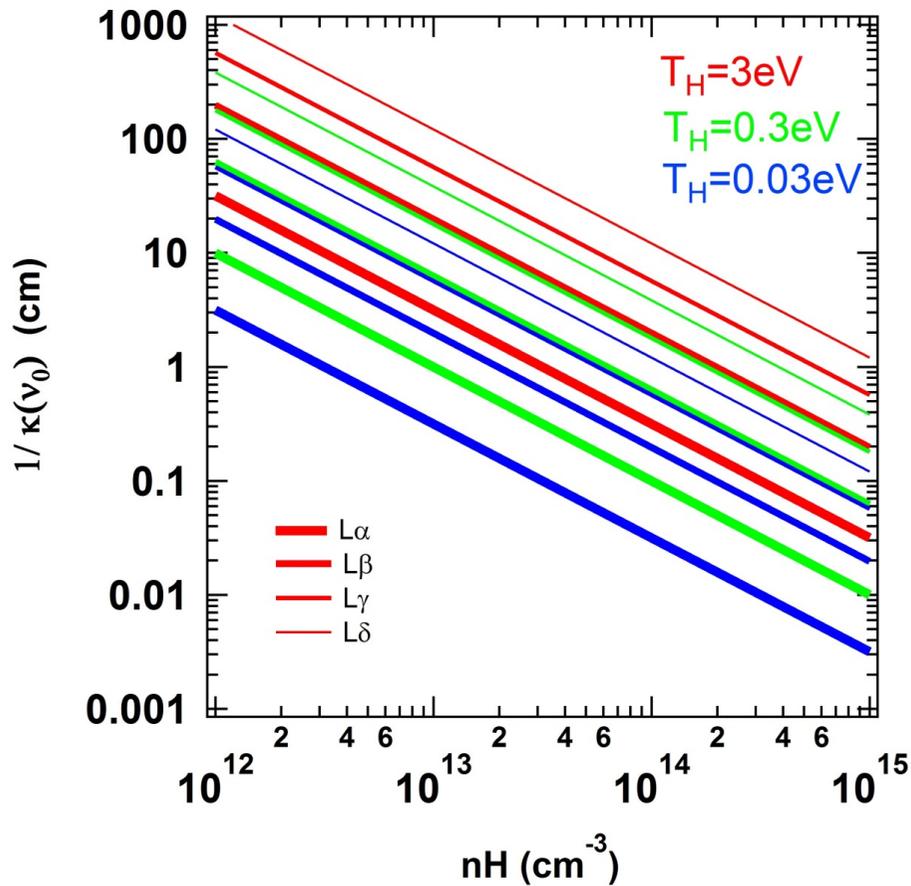
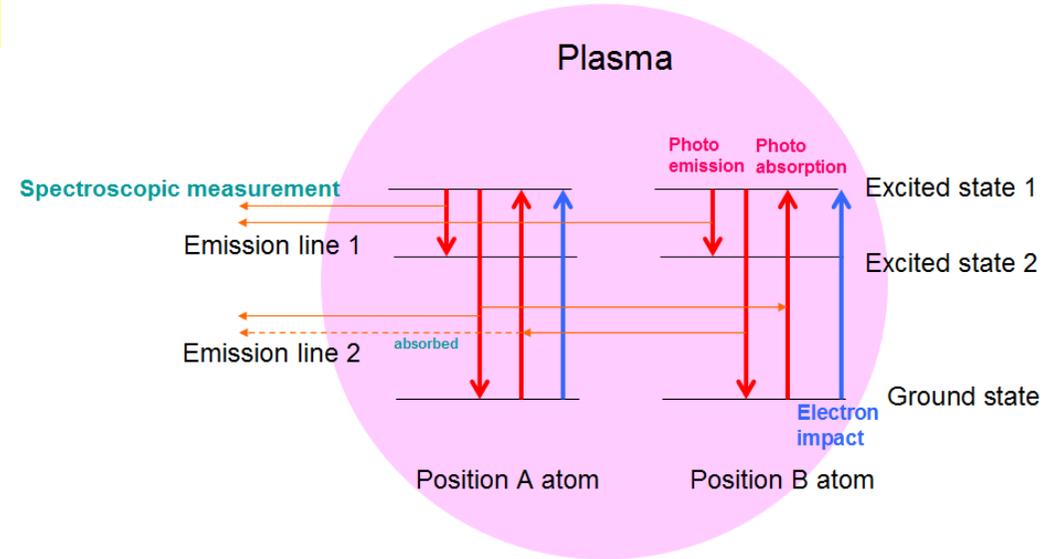
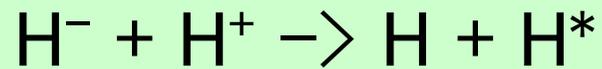
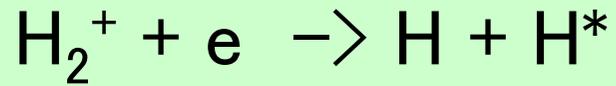
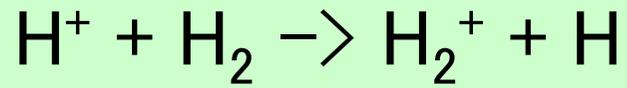


中性粒子輸送コードへの組み込み

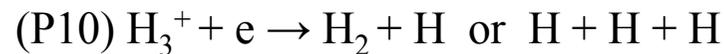
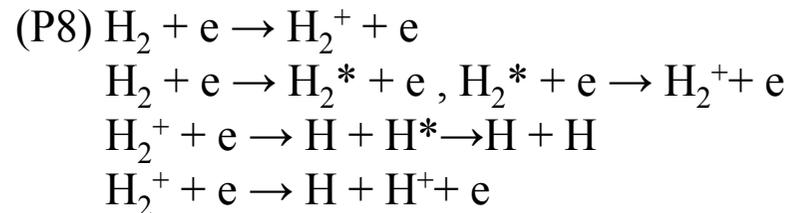
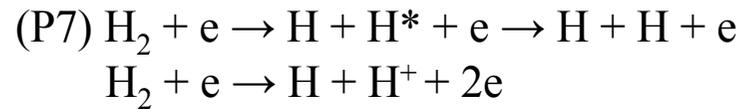
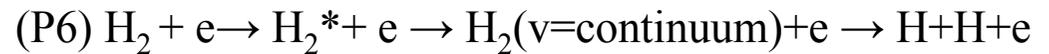
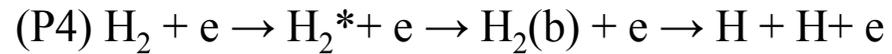
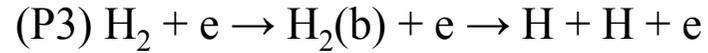
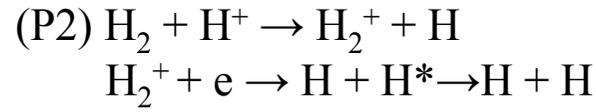
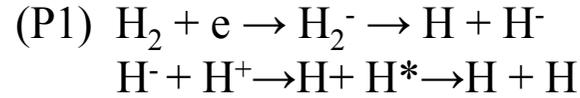
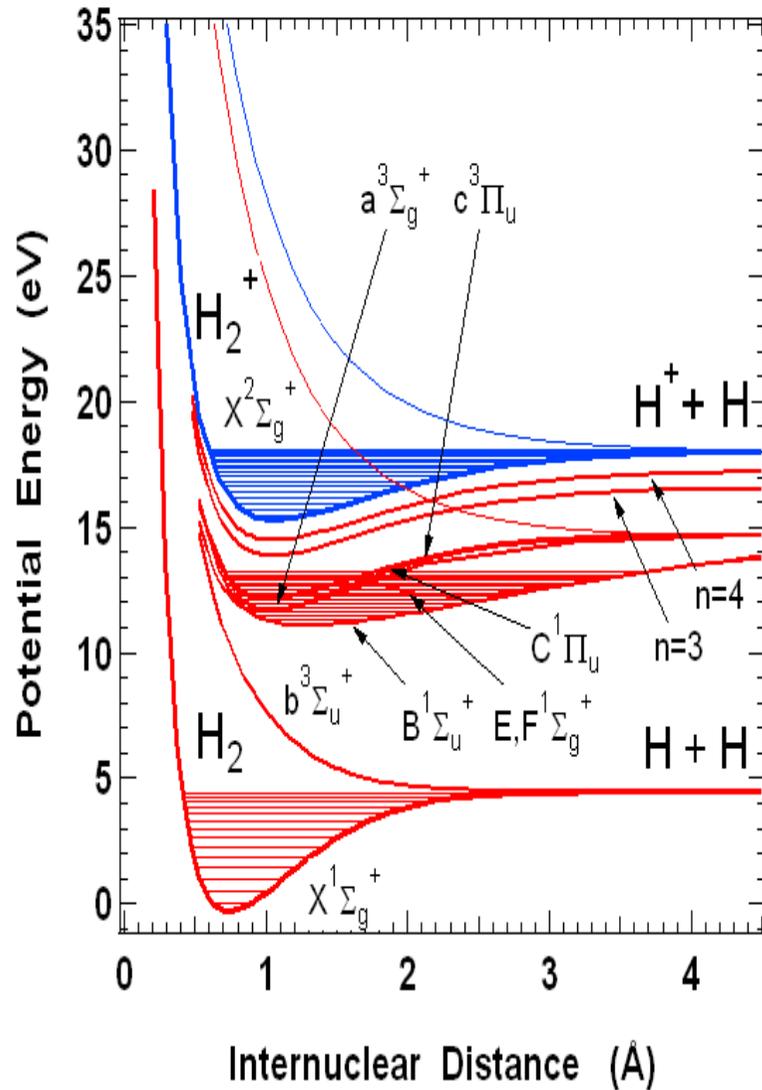
- 水素原子の精密な速度分布
(原子密度, 輻射輸送, 壁に当たる水素原子の速度分布)
- 水素分子の振動回転ポピュレーション

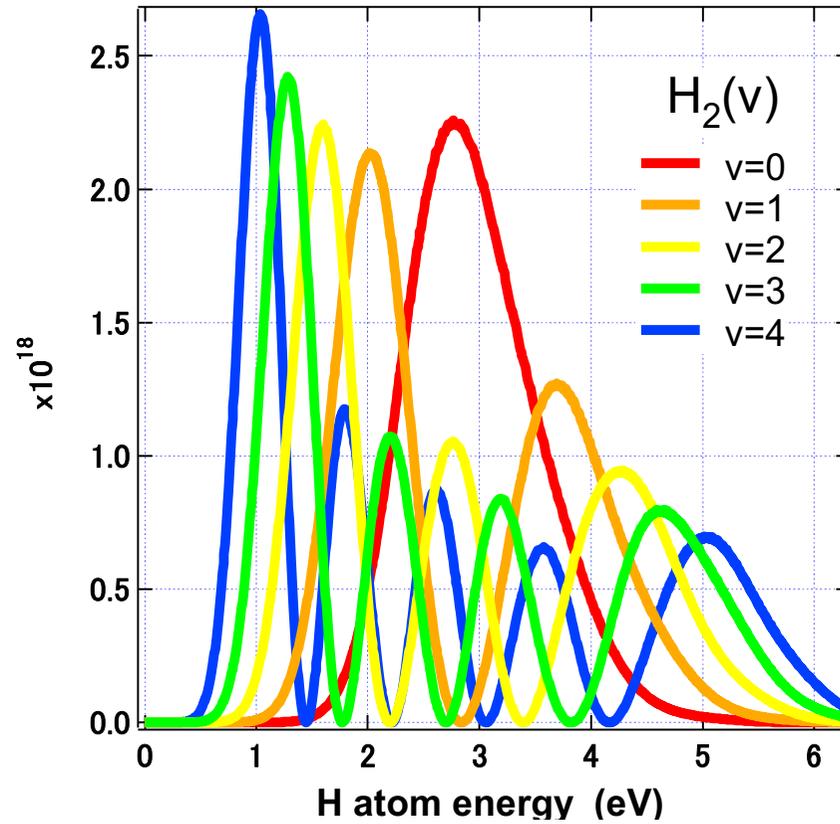
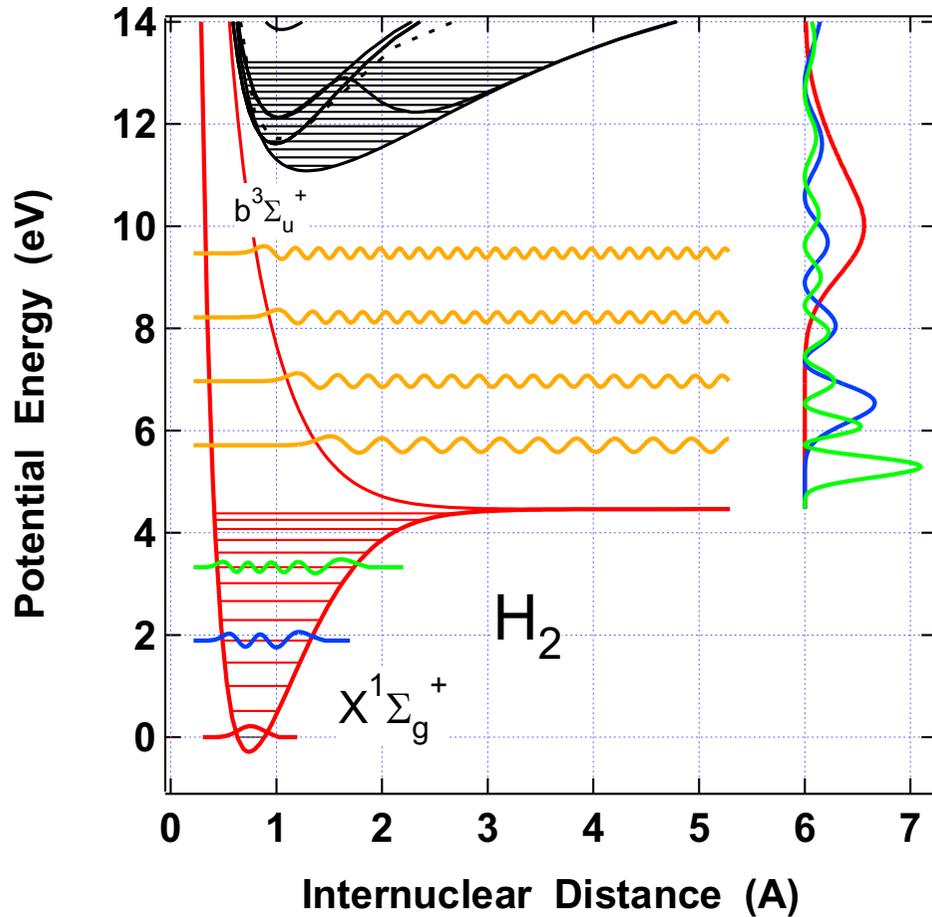


ライマン線吸収長



輸送コードで考慮されている原子生成過程





- ・水素原子生成時のエネルギー
→ 3 eV で多く分布
- ・水素分子
並進温度, 回転温度, 振動温度
= 300 K

$H_2(v, J) + H \rightarrow H_2(v', J') + H$ 中性粒子輸送コードへの組み込み

水素原子エネルギー損失

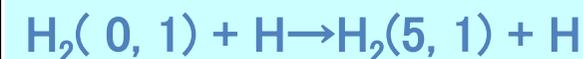
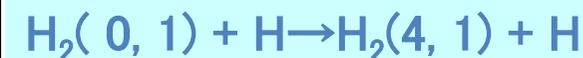
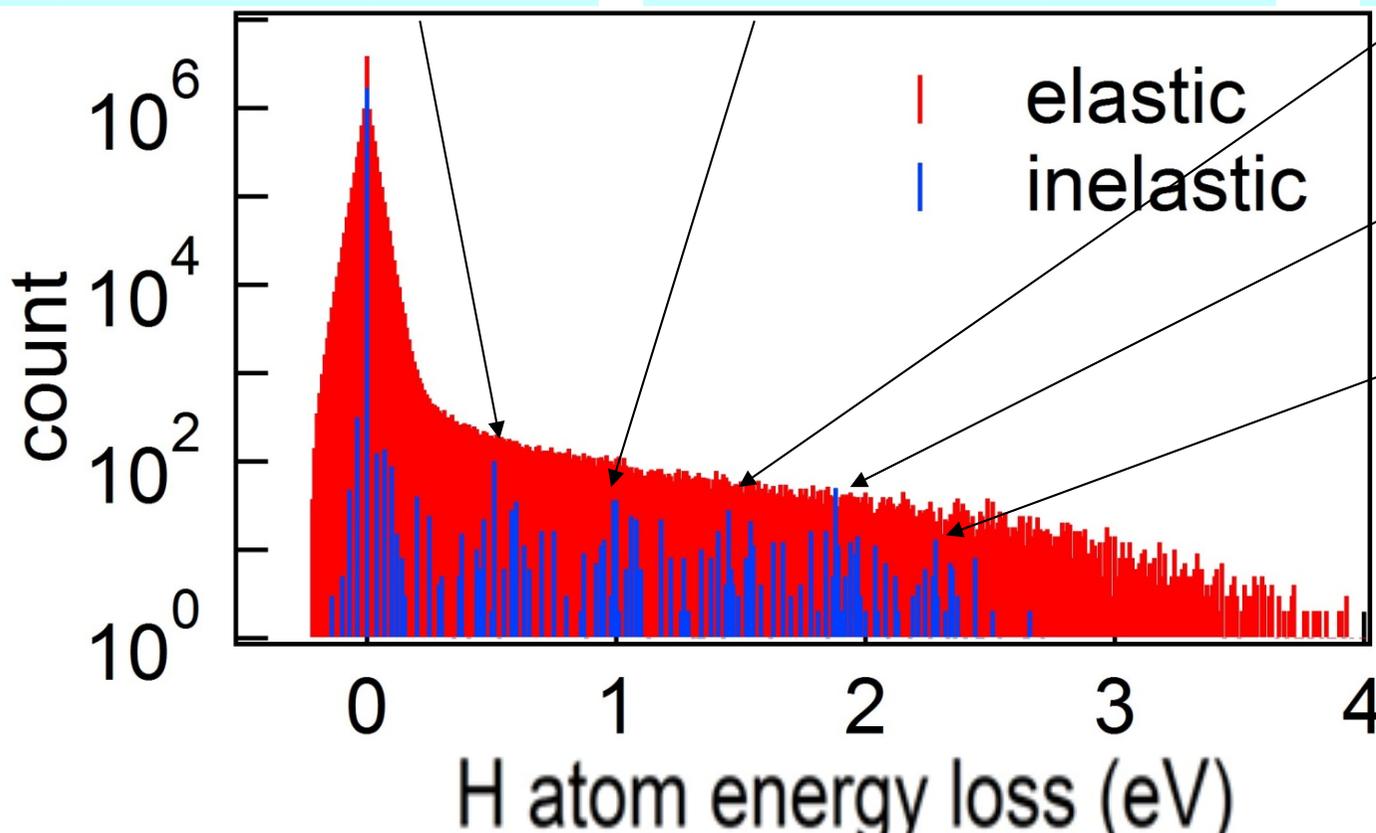
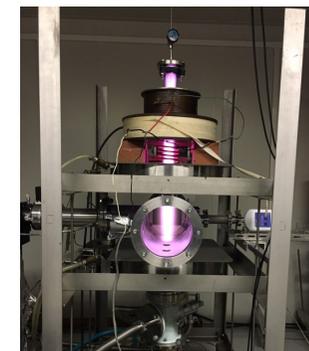
- 分子温度（並進:振動:回転）を300Kで固定
- 相対速度を原子の速度

$$T_e = 3.5 \text{ eV}$$

$$n_e = 4 \times 10^9 \text{ cm}^{-3}$$

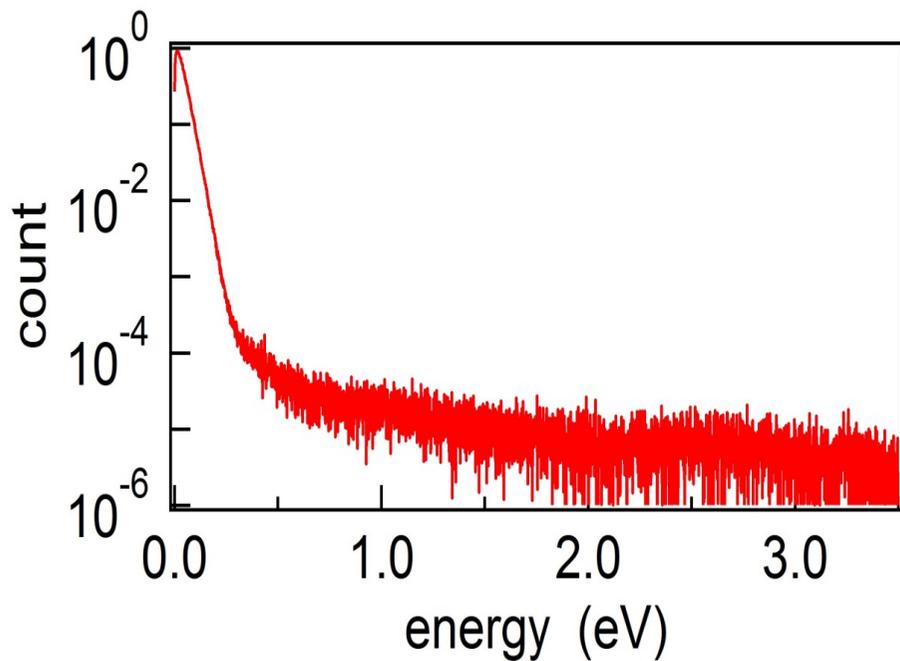
$$T_{H_2} = 300 \text{ K}$$

$$n_{H_2} = 2 \times 10^{15} \text{ cm}^{-3}$$

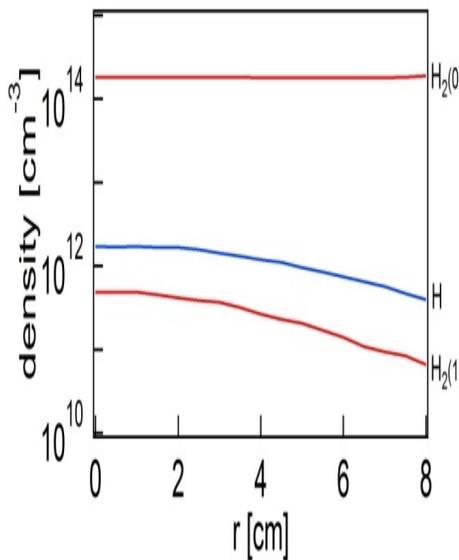
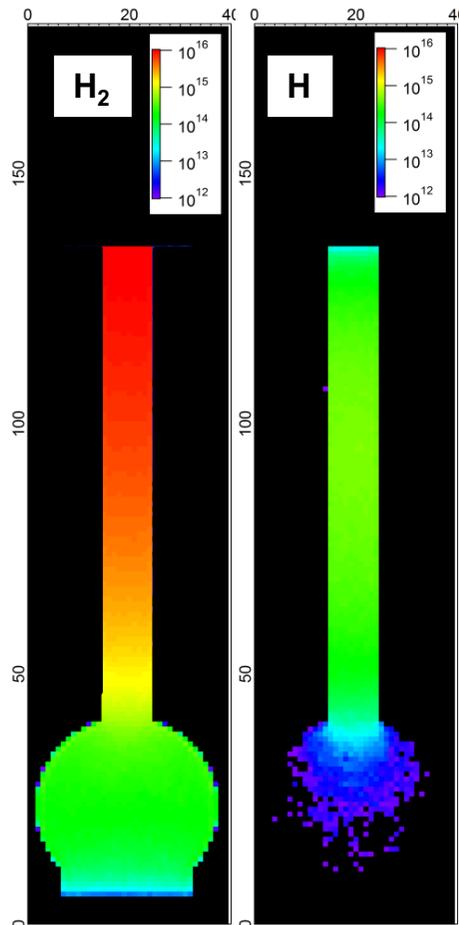
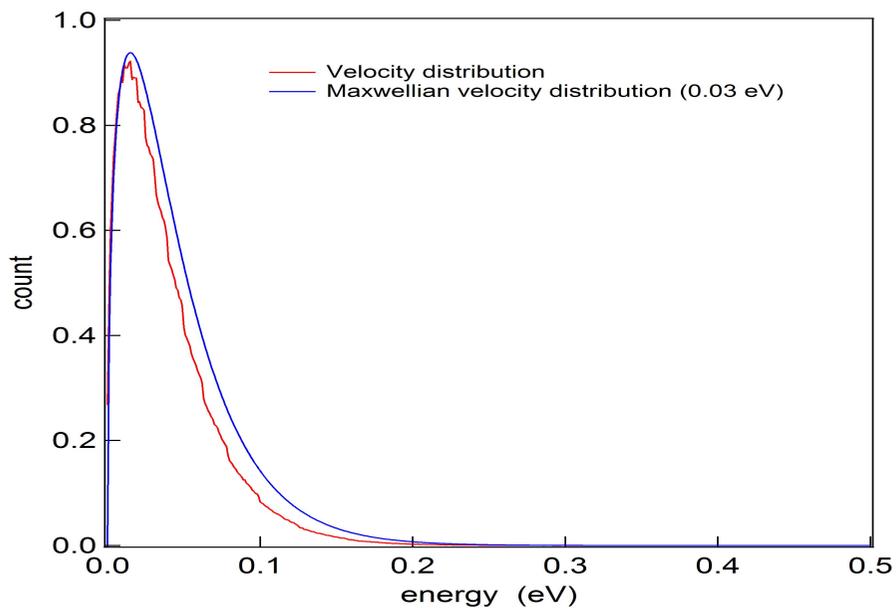


DEMO等、分子と原子の
並進温度が緩和の場合は
非弾性過程
が原子エネルギー損失に
効く可能性あり

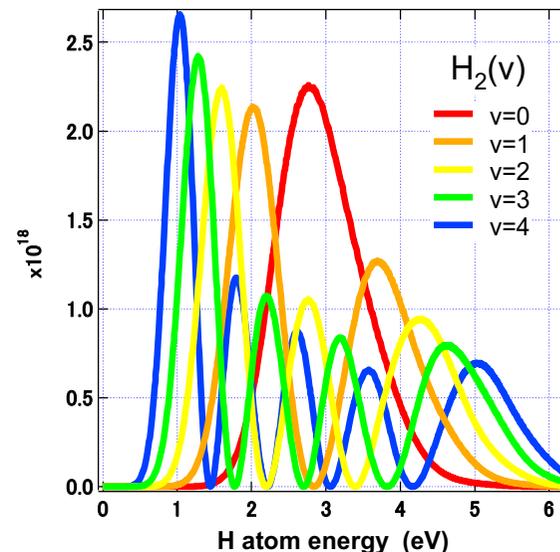
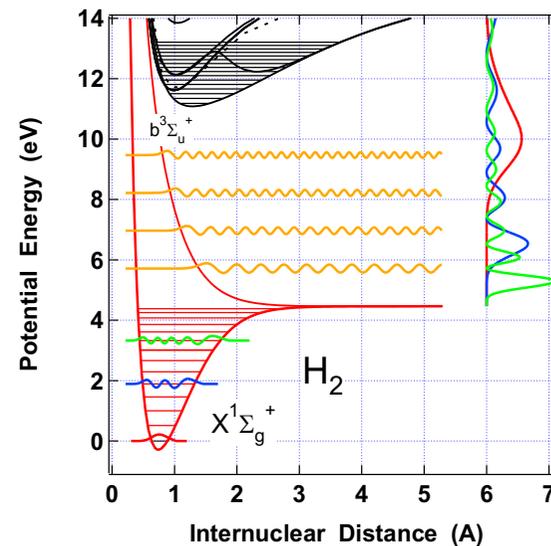
水素原子速度分布



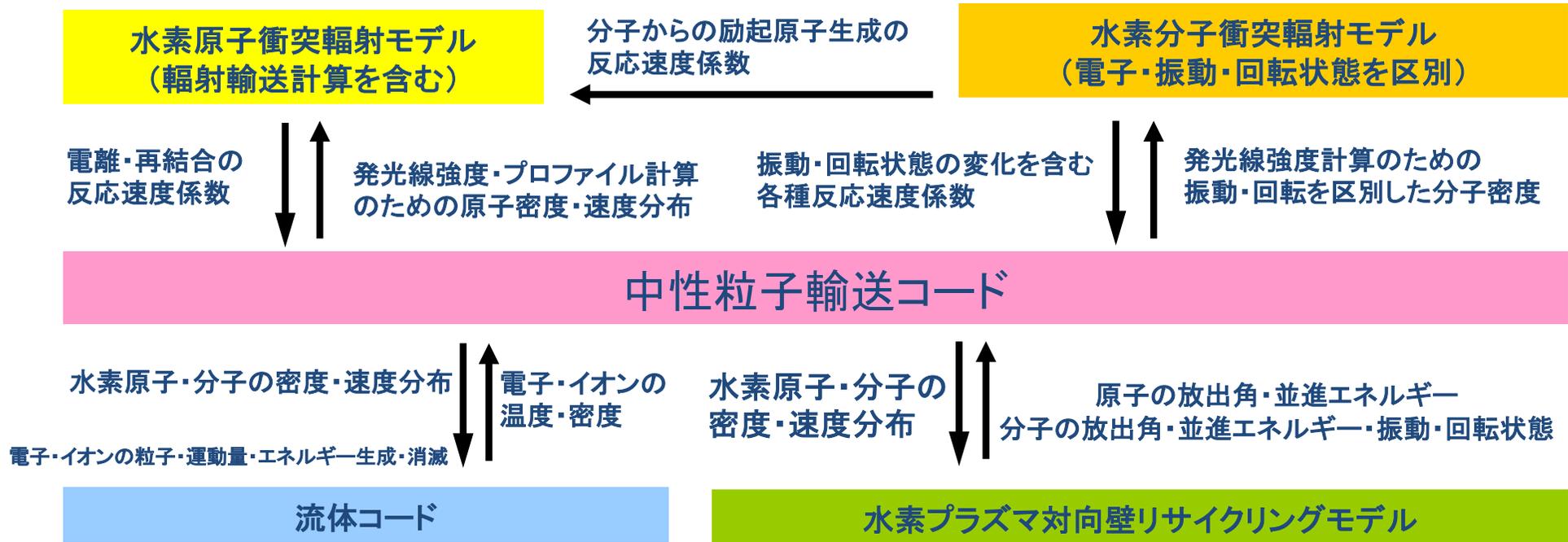
上图扩大



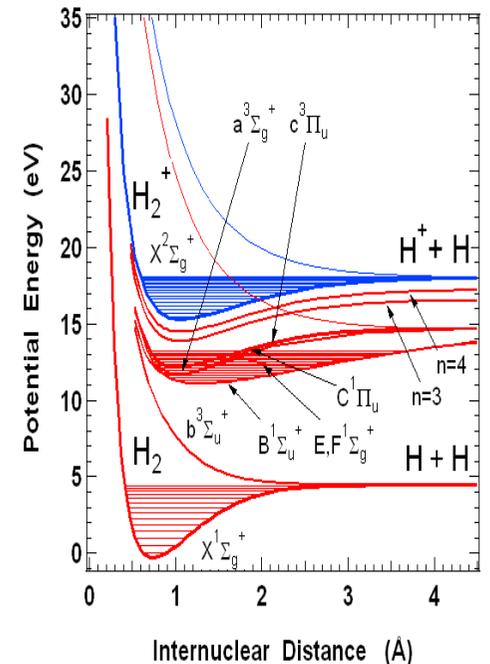
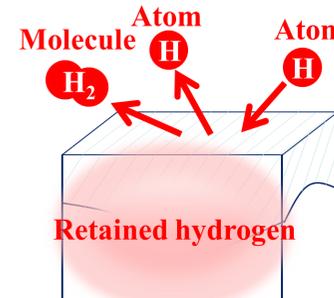
原子生成 $H_2(X) \rightarrow H_2(b) \rightarrow H + H$



水素分子の電子・振動・回転状態を区別したコードの整備



- (1) ダイバータプラズマの水素分子との衝突によるエネルギー損失の計算 (H₂衝突輻射モデル)
- (2) H₂+H による水素原子のエネルギー損失 (中性粒子輸送コード: 信州大RFプラズマ)
- (3) いろいろな壁材における H の反射・再結合の実験
- (4) HD衝突輻射モデルの構築

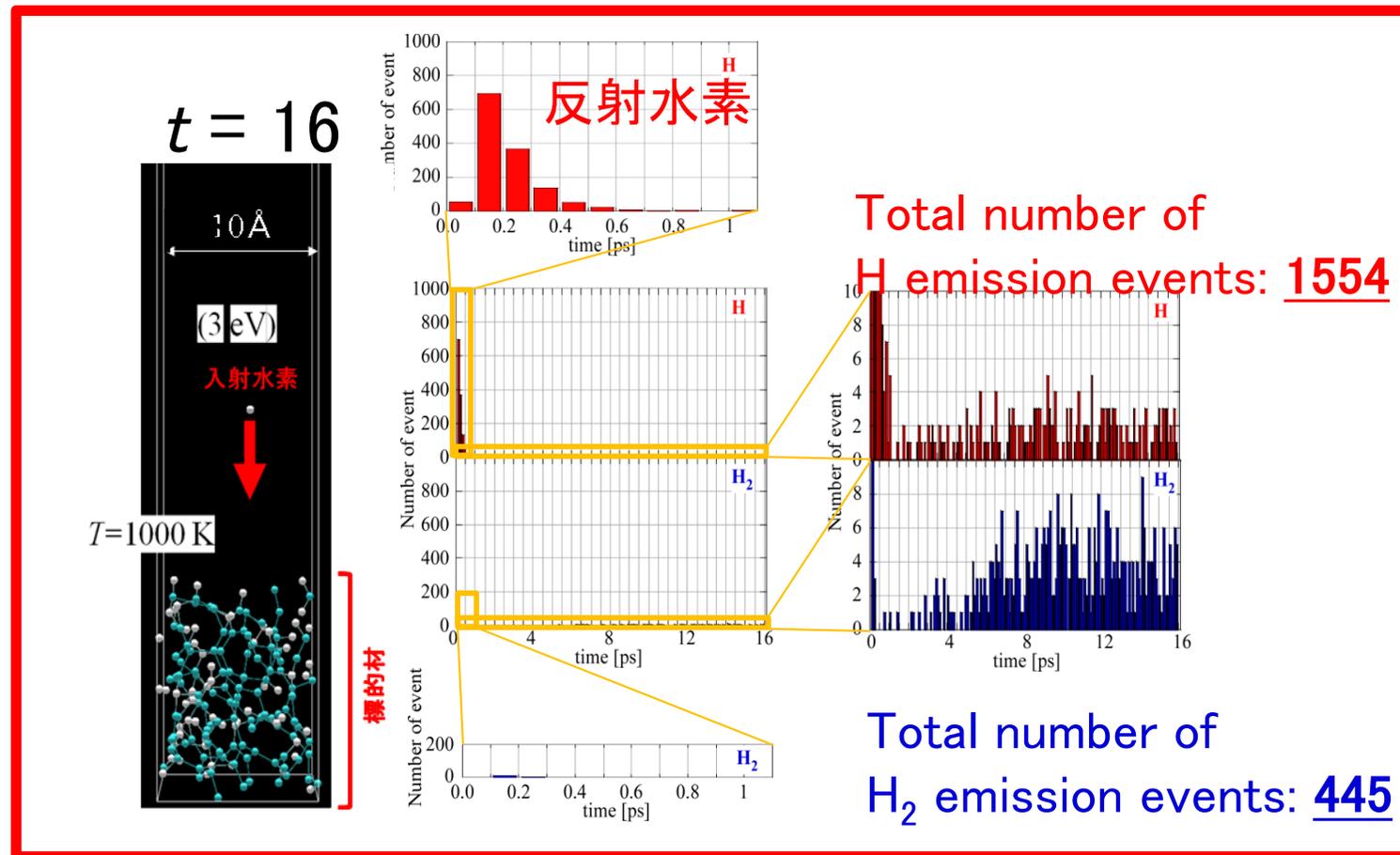


水素プラズマ対向壁リサイクリングモデルの構築

NIFS 中村浩章

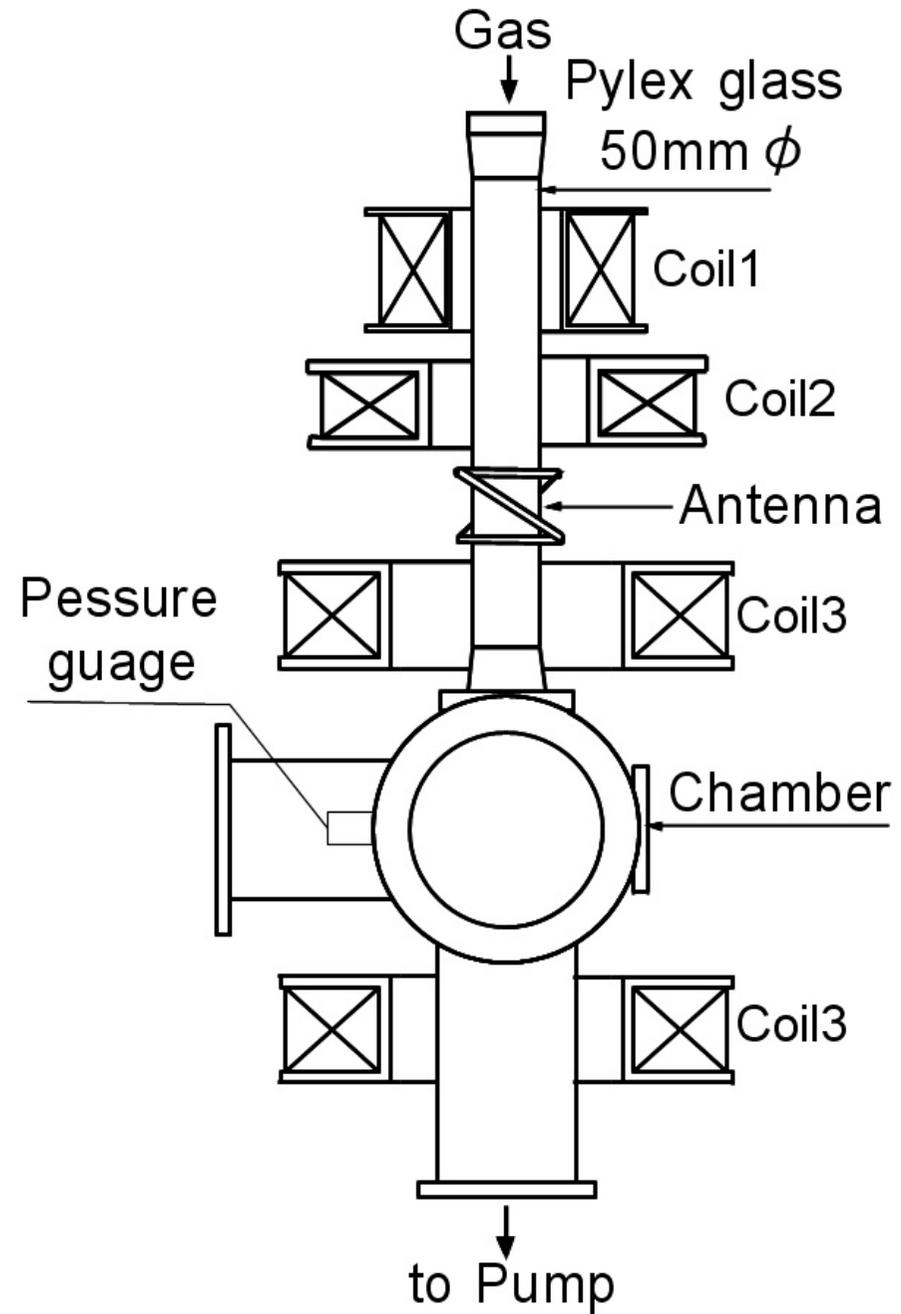
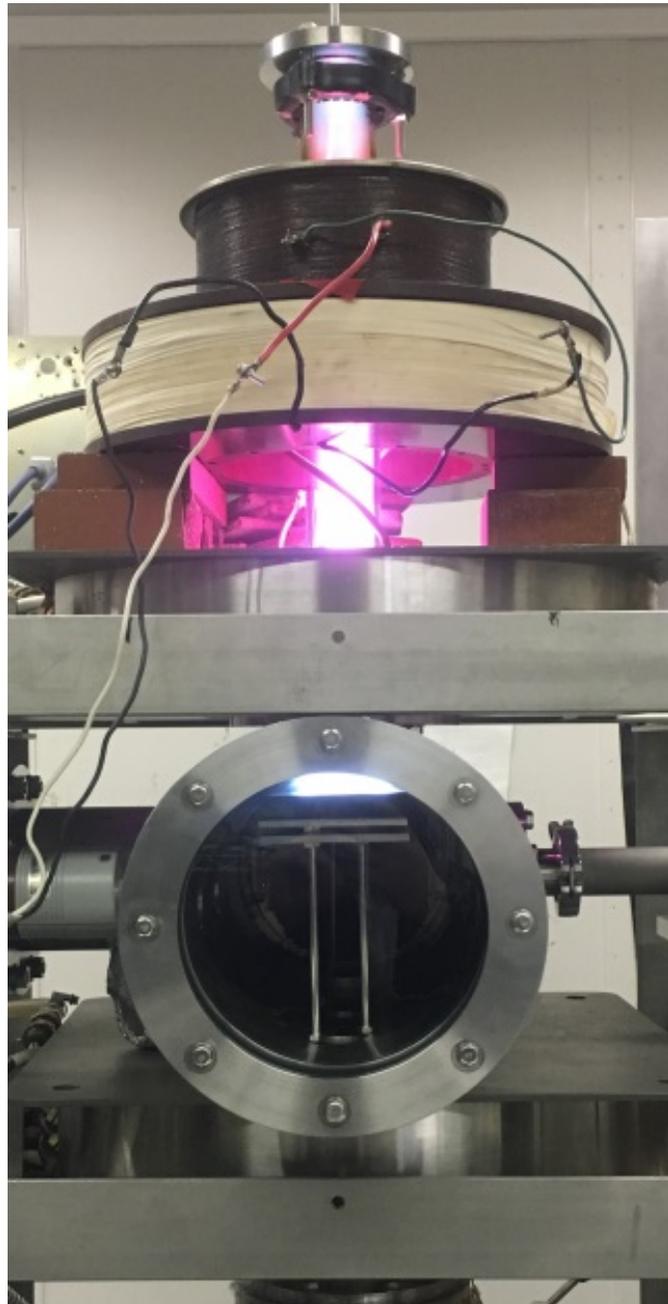
釧路高専

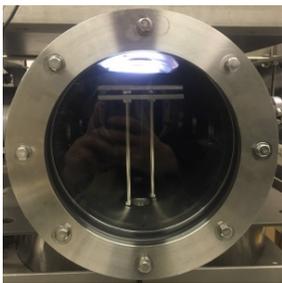
斎藤誠紀



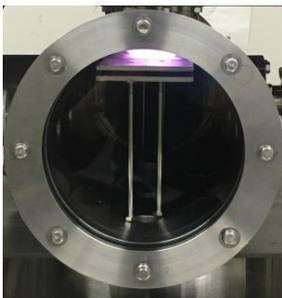
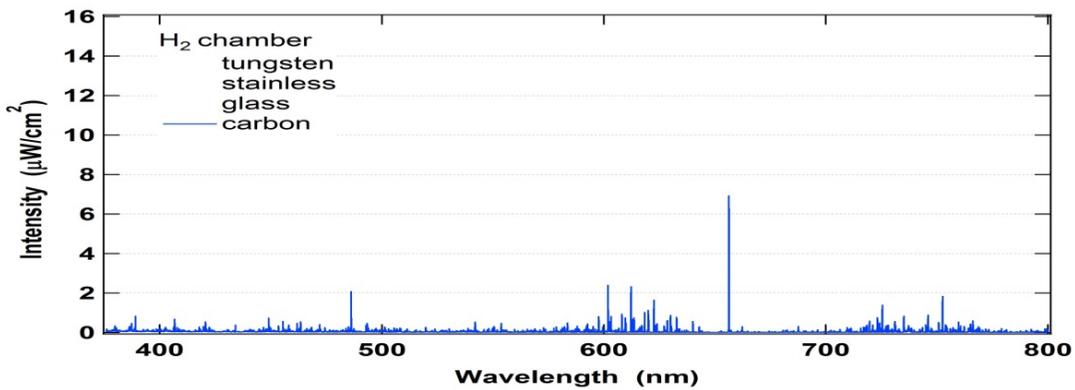
分子動力学を用いたプラズマ対向壁シミュレーションの検証のための
炭素板・ステンレス板・タングステン板・ガラス板近傍プラズマの分光計測

実験装置

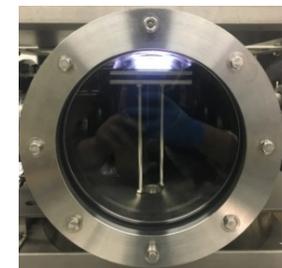
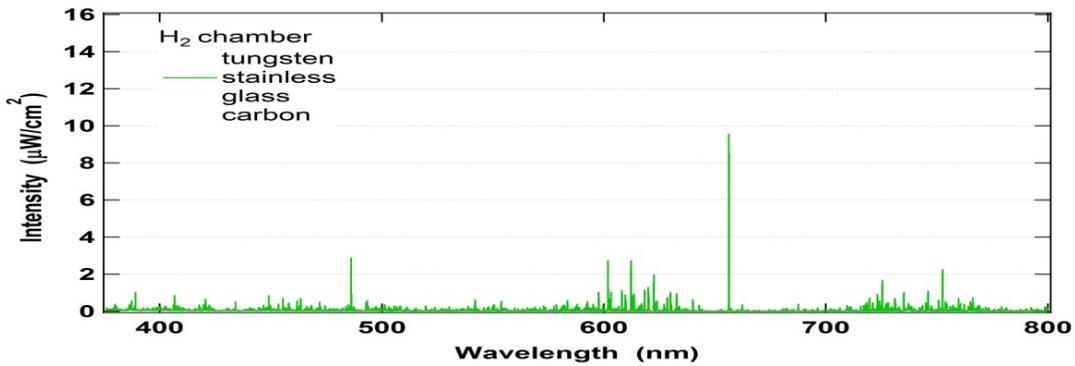




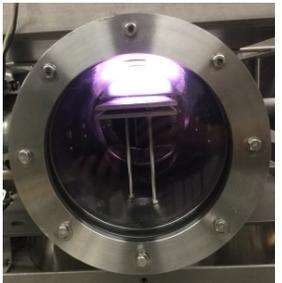
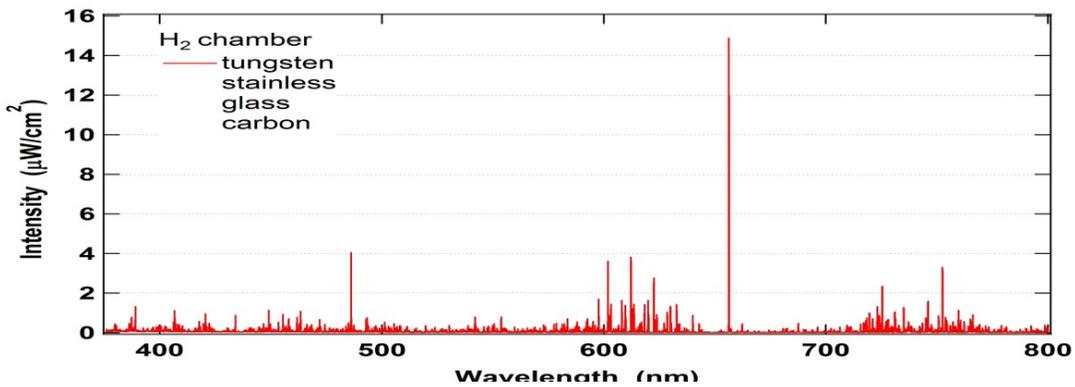
カーボン板



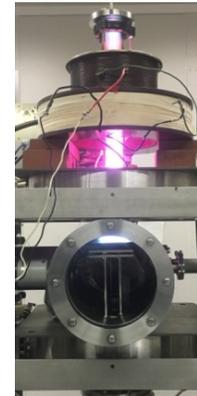
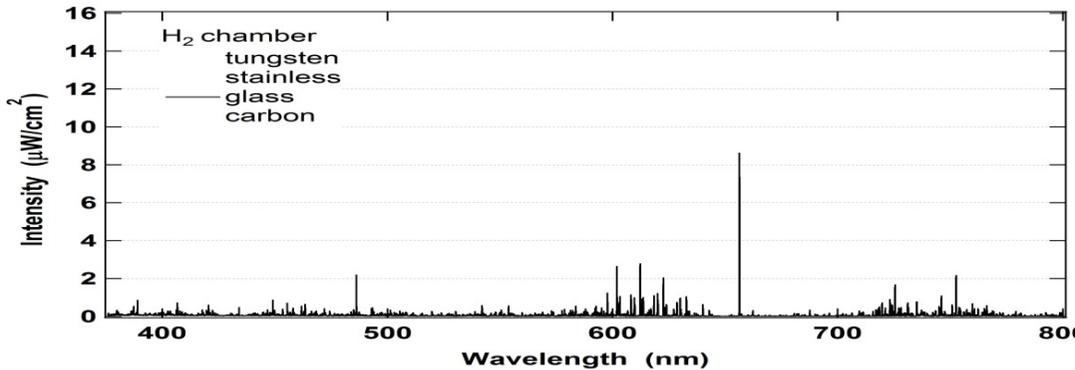
ステンレス板



タングステン板

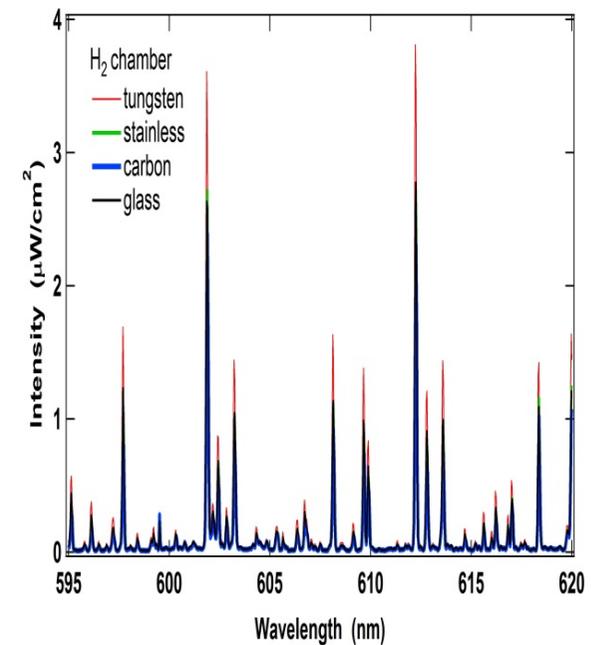
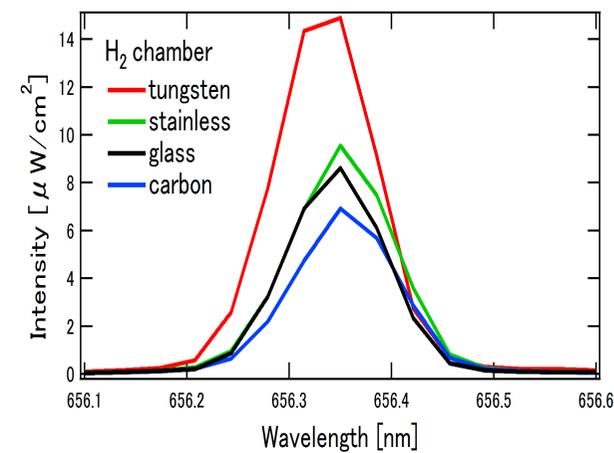


ガラス板

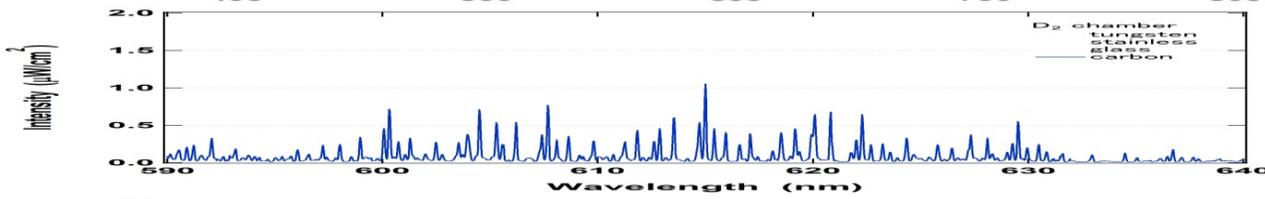
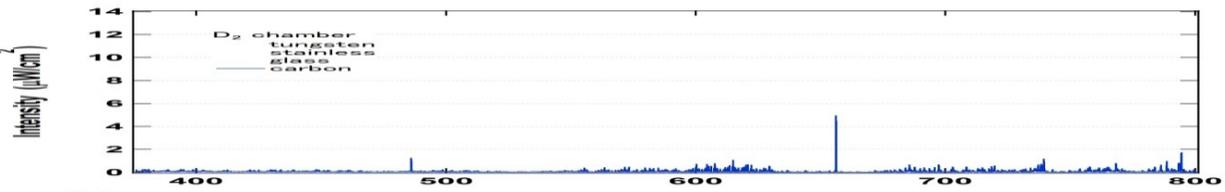


H₂ チャンバー部分 分光計測

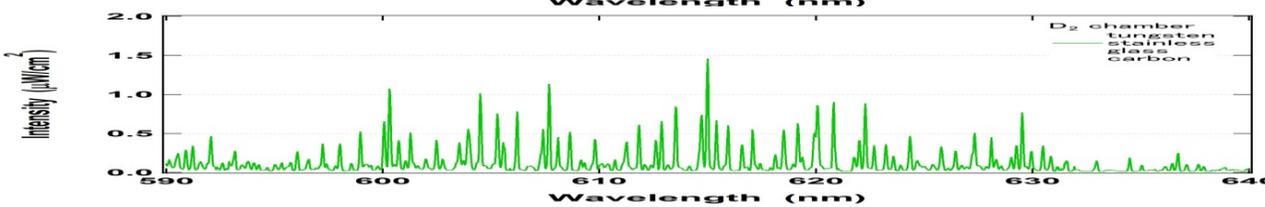
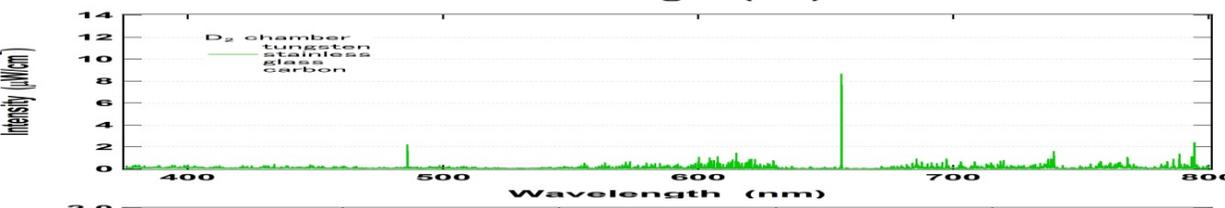
H₂ 0.02 Torr
アンテナ出力1500 W



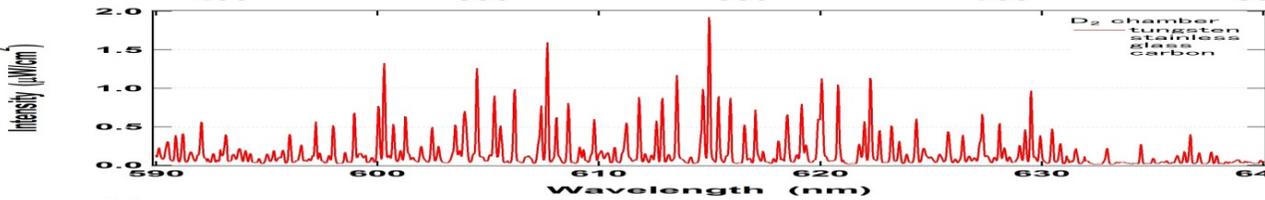
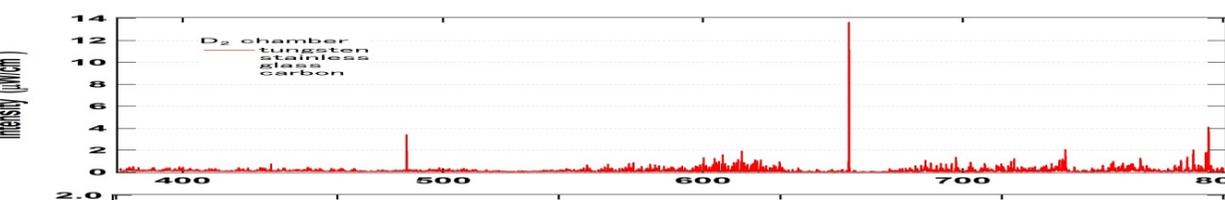
カーボン板



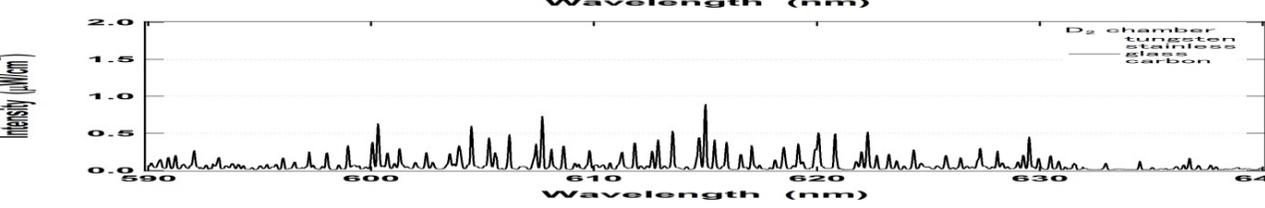
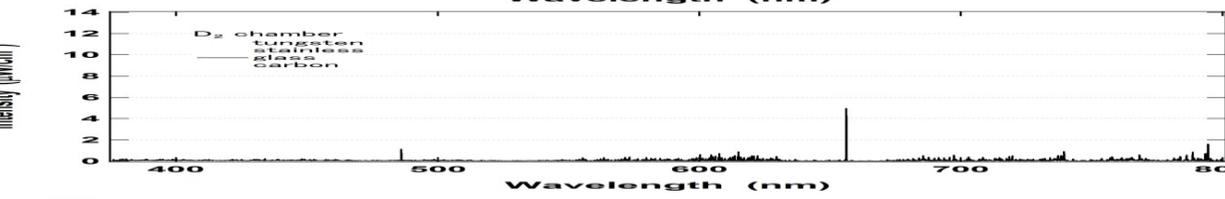
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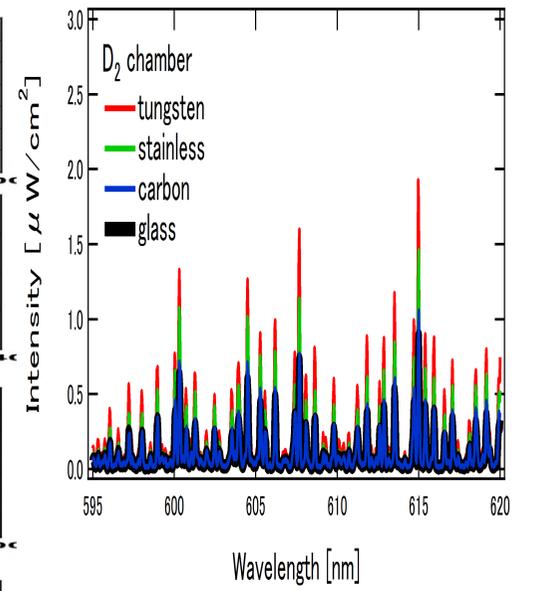
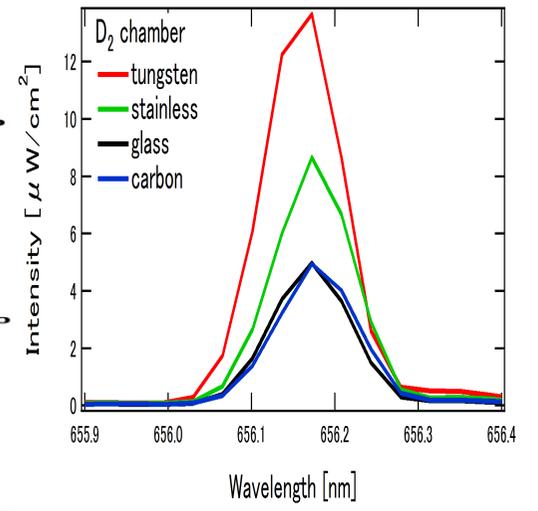
タングステン板



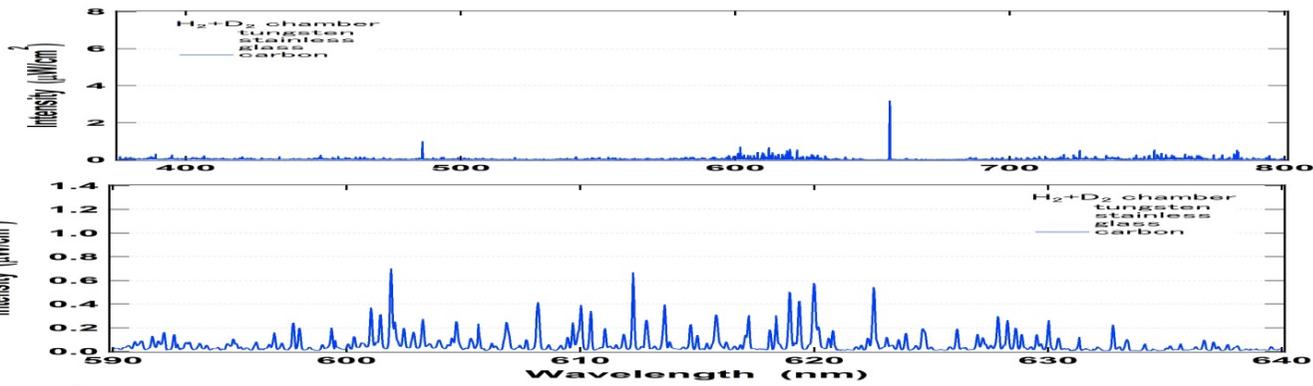
ガラス板



D₂ チャンバー部分光計測
D₂ 0.02 Torr
アンテナ出力 1500 W



カーボン板

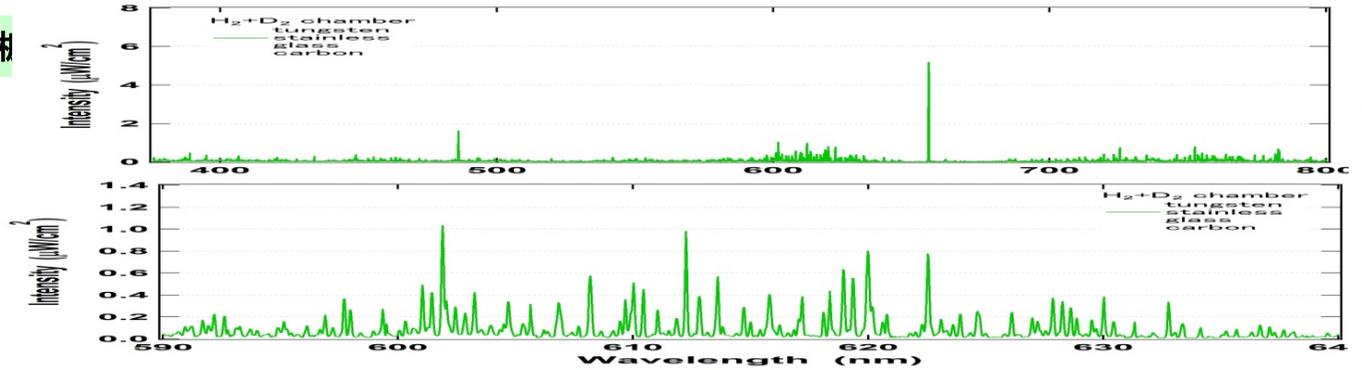


H₂+D₂ チャンバー部
分光計測

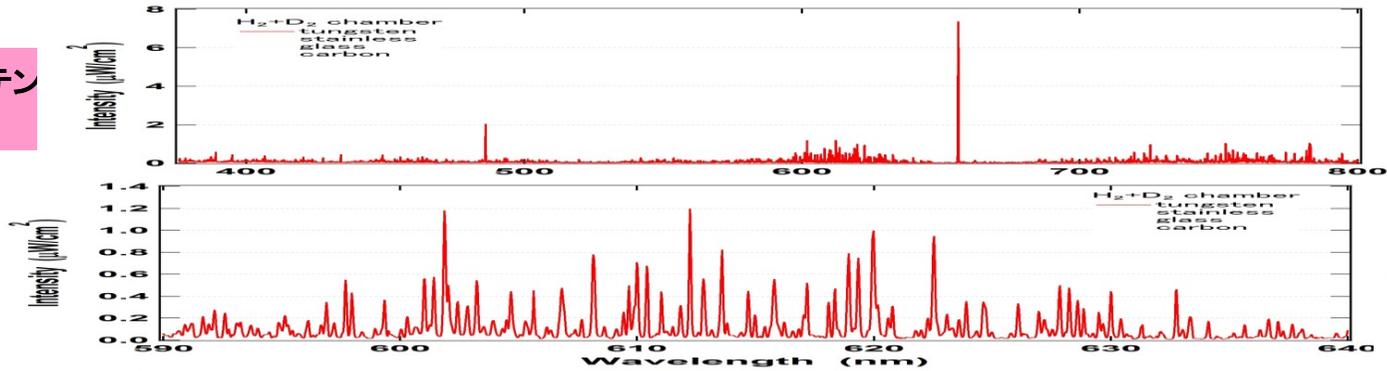
H₂ 0.01 Torr
D₂ 0.01 Torr

アンテナ出力 1500 W

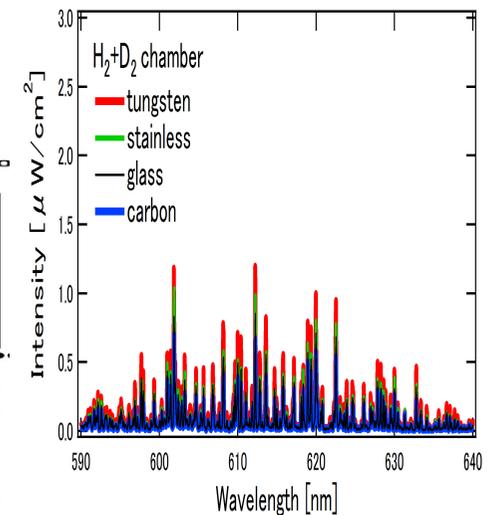
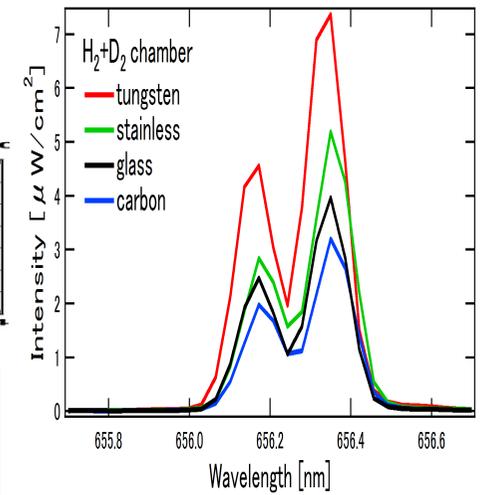
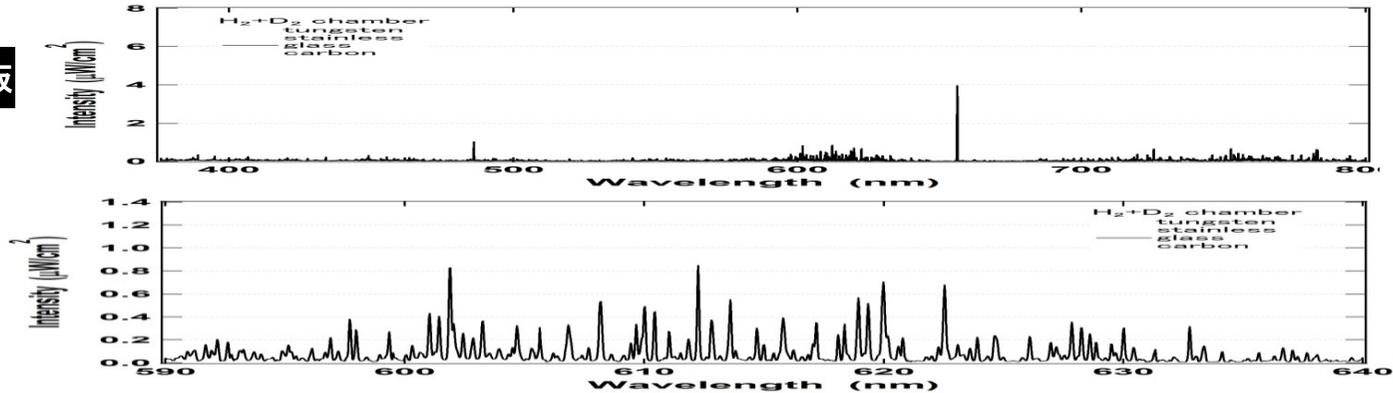
ステンレス材



タングステン
板



ガラス板



RECOMBINATION COEFFICIENTS OF HYDROGEN ATOMS ON VARIOUS METAL SURFACES AS A FUNCTION OF TEMPERATURE

| Probe surface | Surface temp., °K. | γ' |
|---------------|--------------------|-----------|
| W | 353 | 0.065 |
| | 423 | .055 |
| | 533 | .068 |
| | 563 | .062 |
| | 573 | .055 |
| | 578 | .054 |
| | 643 | .059 |
| | 678 | .062 |
| | 723 | .057 |
| | 923 | .062 |
| | 1088 | .067 |
| Cu | 333 | .14 |
| | 543 | .10 |
| | 693 | .10 |
| Al | 328 | .29 |
| | 328 | .32 |
| | 423 | .21 |
| | 733 | .27 |
| Ti | 308 | .35 |
| | 308 | .40 |
| | 335 | .48 |
| | 421 | .35 |
| | 558 | .35 |
| Ni | 303 | .25 |
| | 358 | .13 |
| | 473 | .19 |
| | 623 | .17 |
| | 873 | .14 |
| | Pd | 448 |
| 448 | | .073 |
| 673 | | .052 |
| 763 | | .086 |

水素原子 壁での再結合係数データ

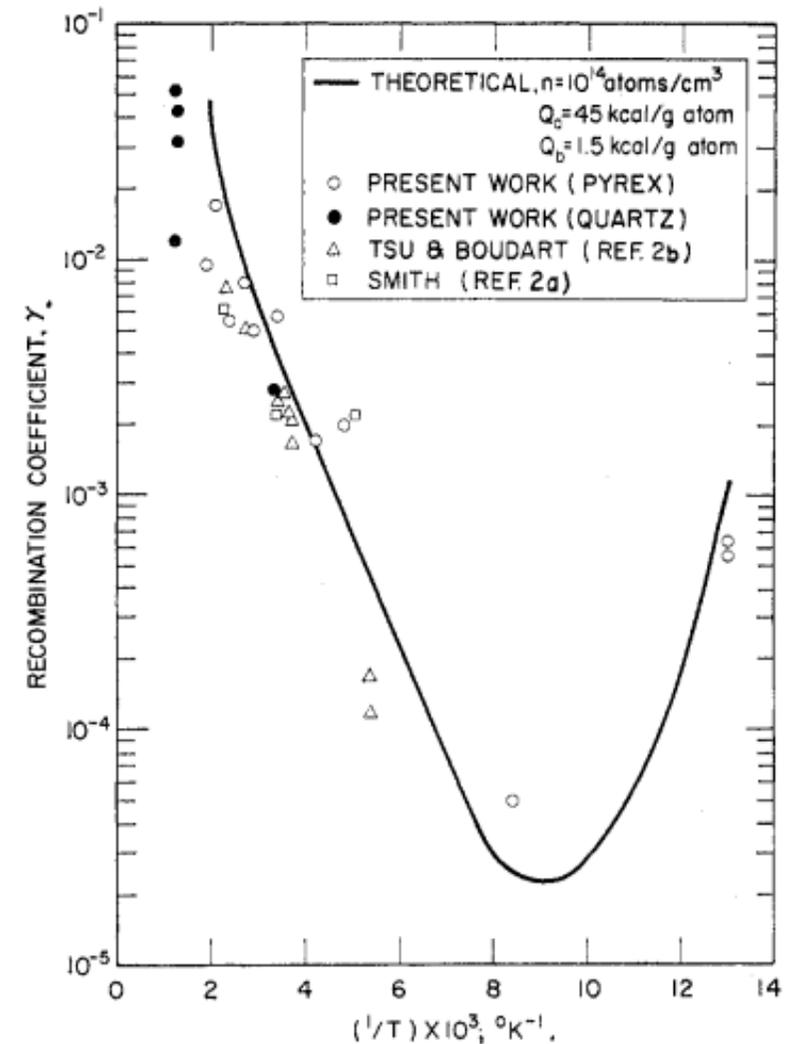


Fig. 3.—Temperature dependence of rate of hydrogen atom recombination on Pyrex glass and fused quartz surfaces. γ_2 calculated for $n = 10^{14}$ atoms/cm.³ from measured second-order rate constants.

THE KINETICS OF HYDROGEN ATOM RECOMBINATION ON PYREX GLASS AND FUSED QUARTZ

Bernard J. Wood, Henry Wise, J. Phys. Chem. 66, 1049–1053 (1962).

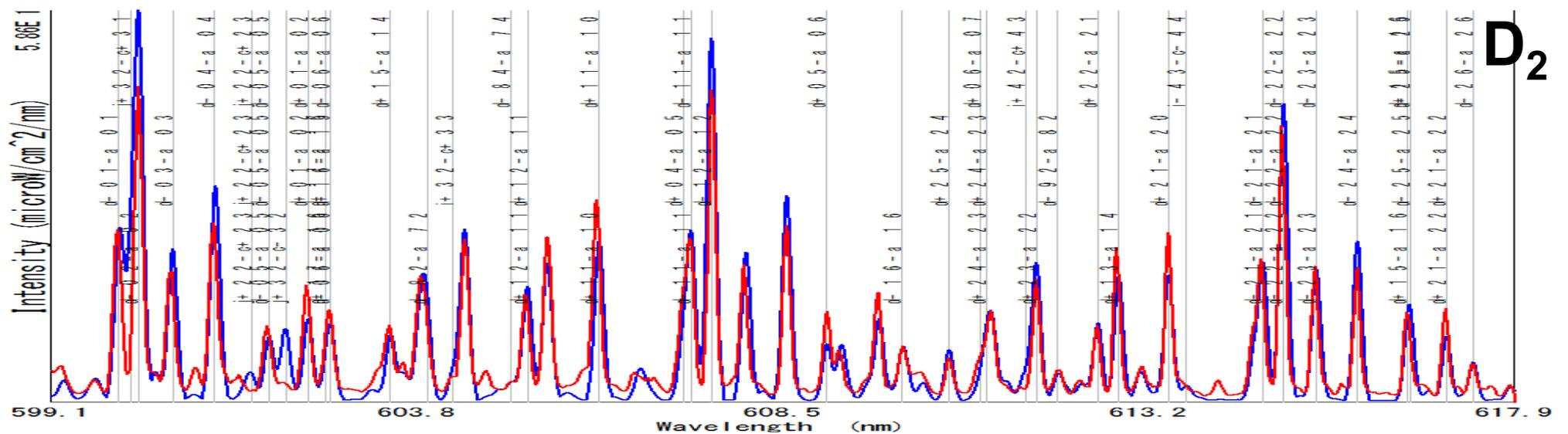
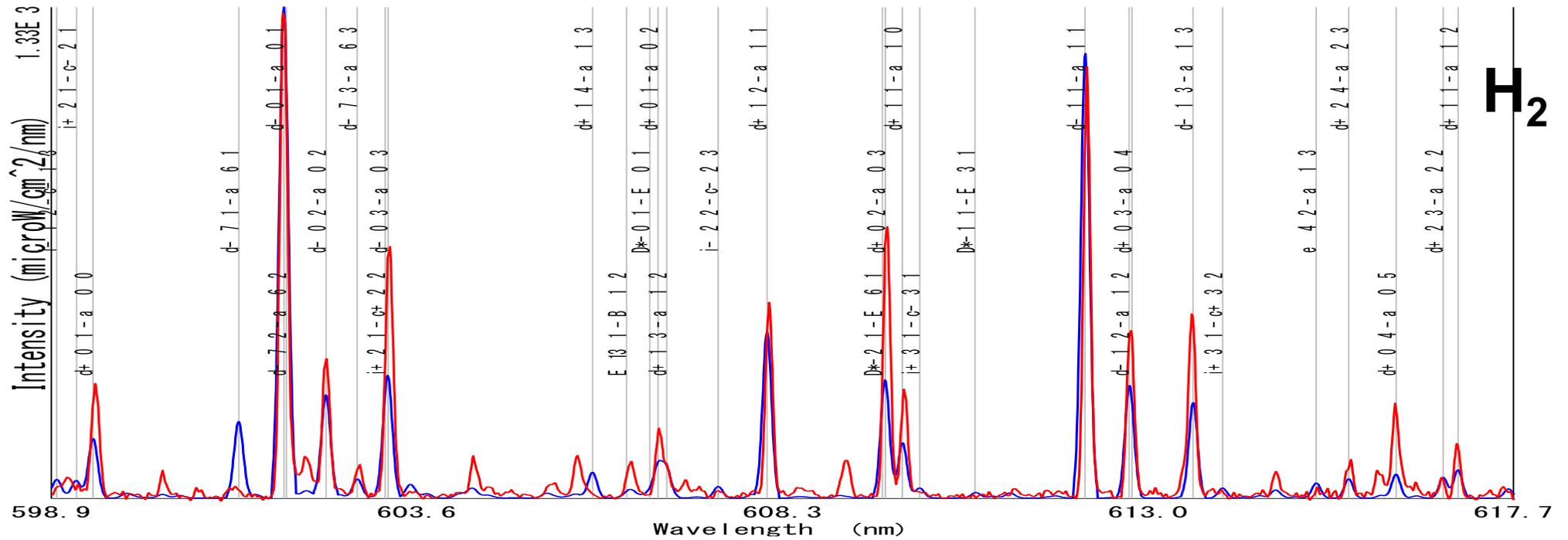
KINETICS OF HYDROGEN ATOM RECOMBINATION ON SURFACES

Bernard J. Wood, Henry Wise, J. Phys. Chem., 1976–1983 (1961).

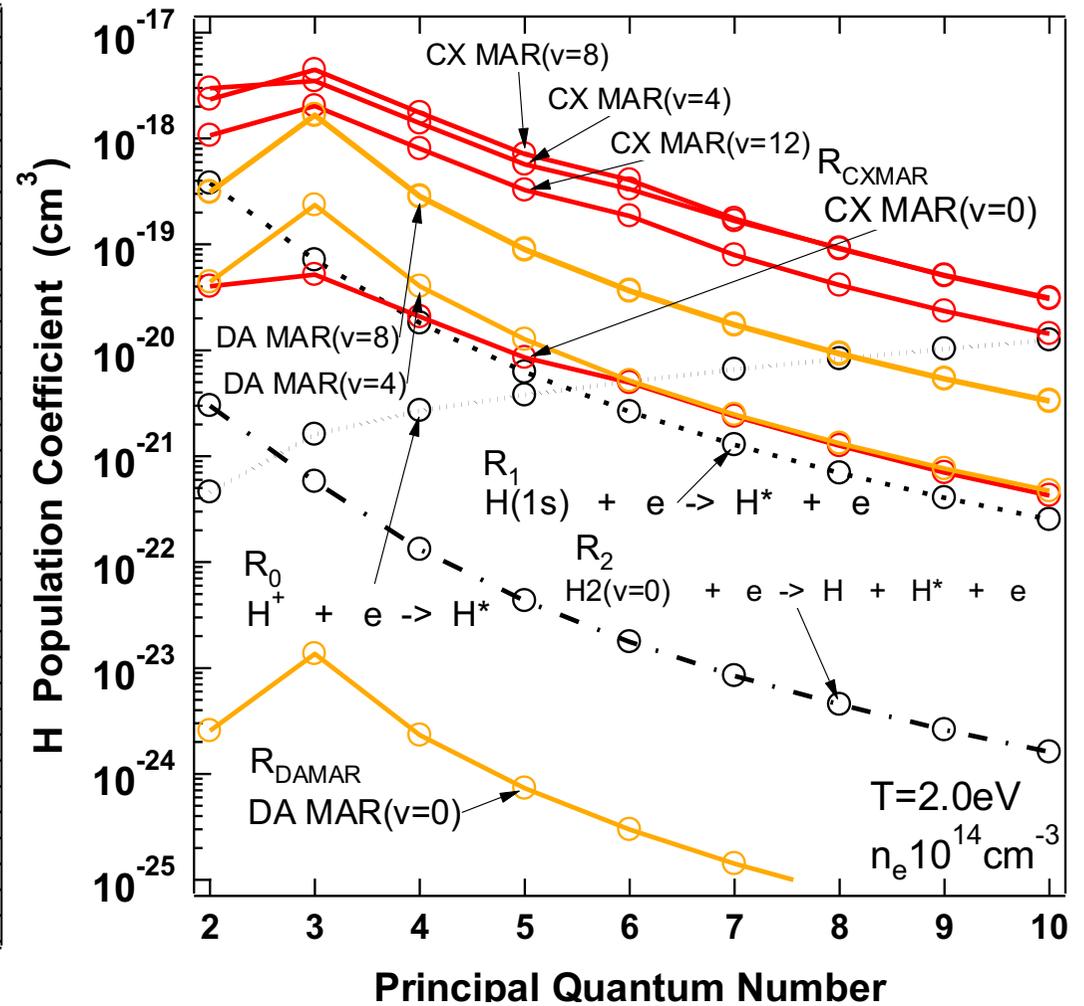
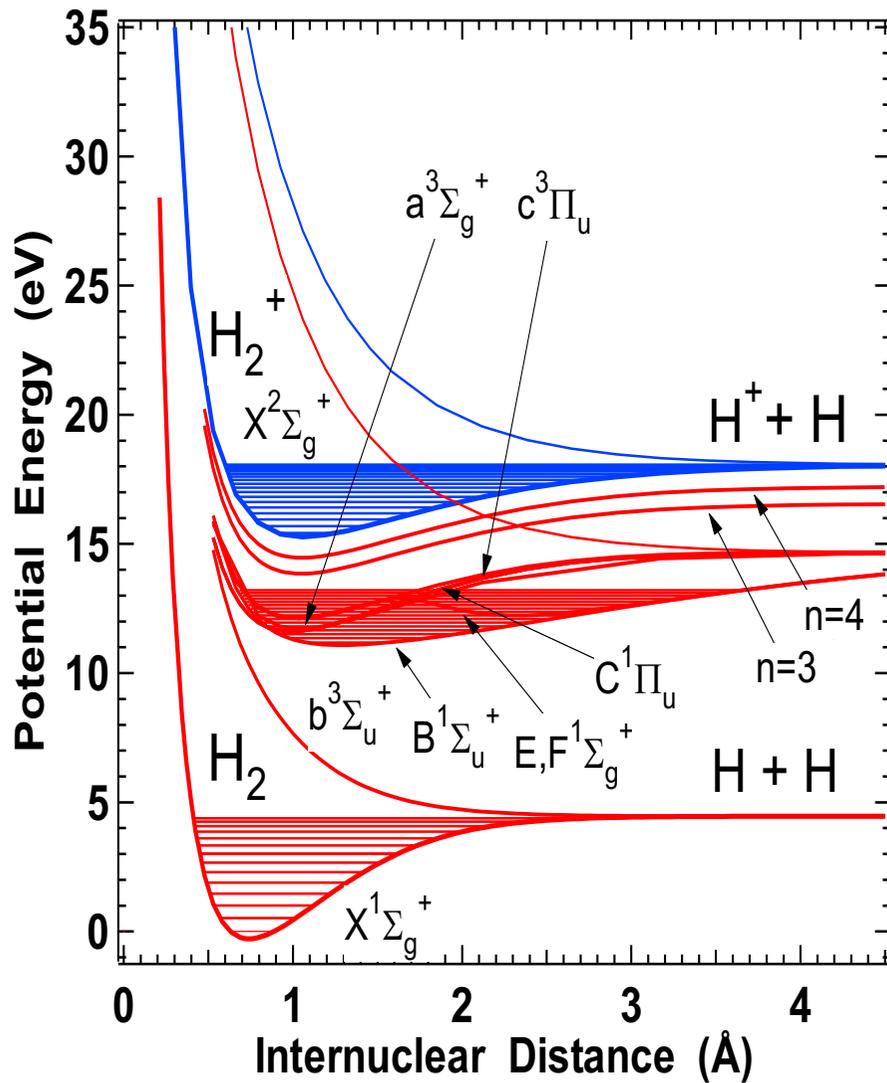
電子温度・密度→分子密度 振動・回転密度分布の解析

H₂ and D₂ Collisional-radiative model

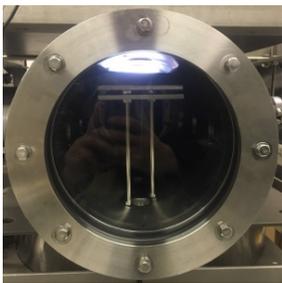
赤: 実験 青: 計算



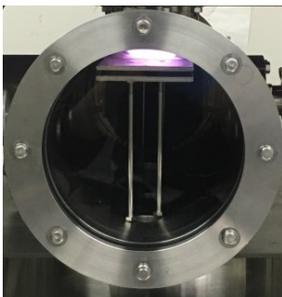
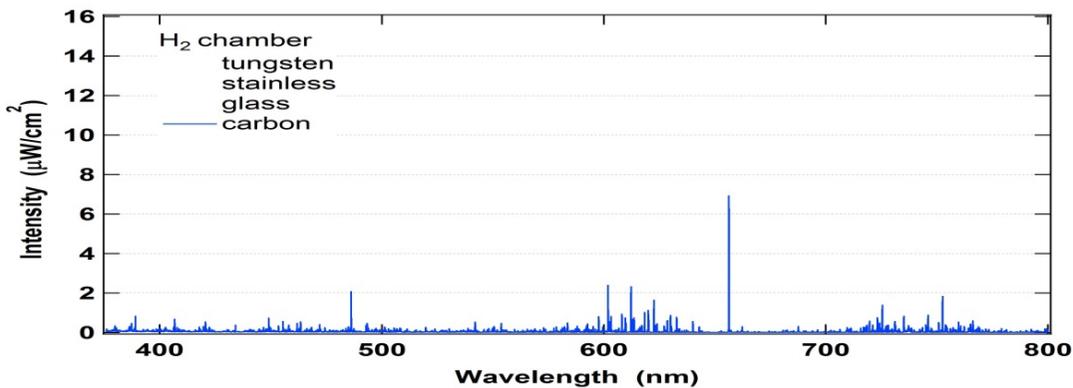
水素原子の発光線強度の解析



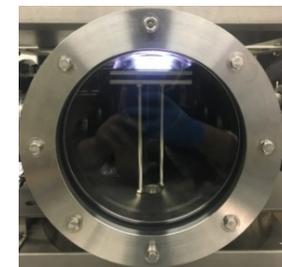
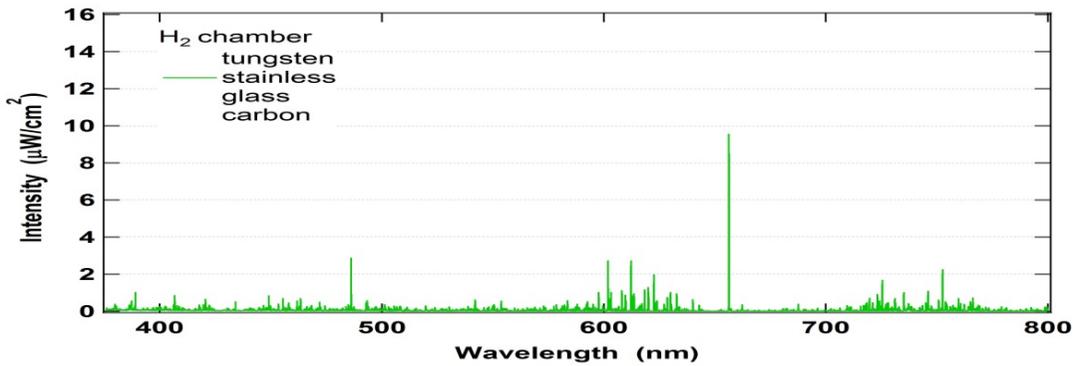
$$n(p) = R_0(p)n_e n_{H^+} + R_1(p)n_e n_H + R_2(p)n_e n_{H_2} + R_{\text{MAR}}(p)n_e n_{H_2} + \text{輻射輸送}$$



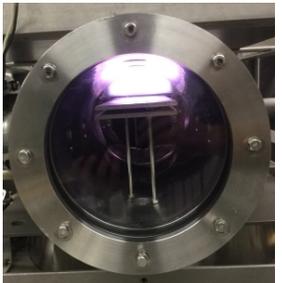
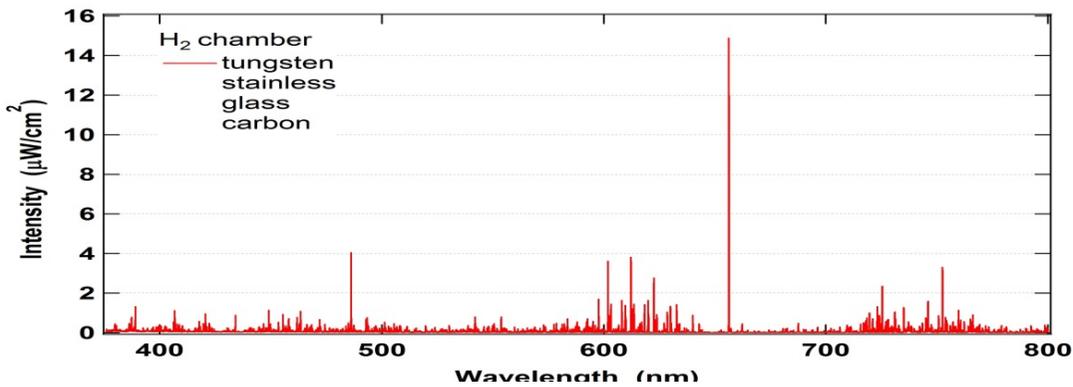
カーボン板



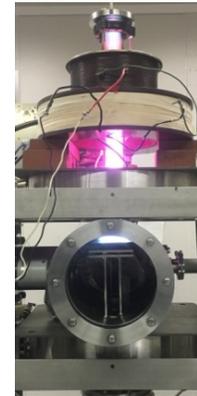
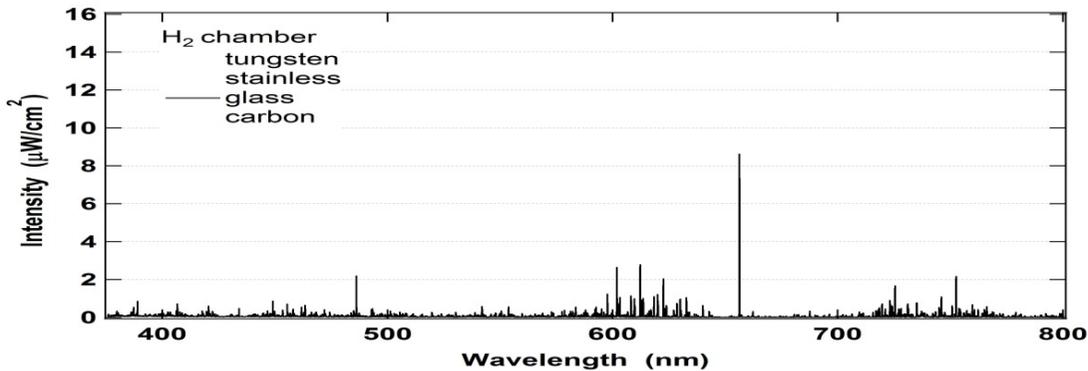
ステンレス板



タングステン板

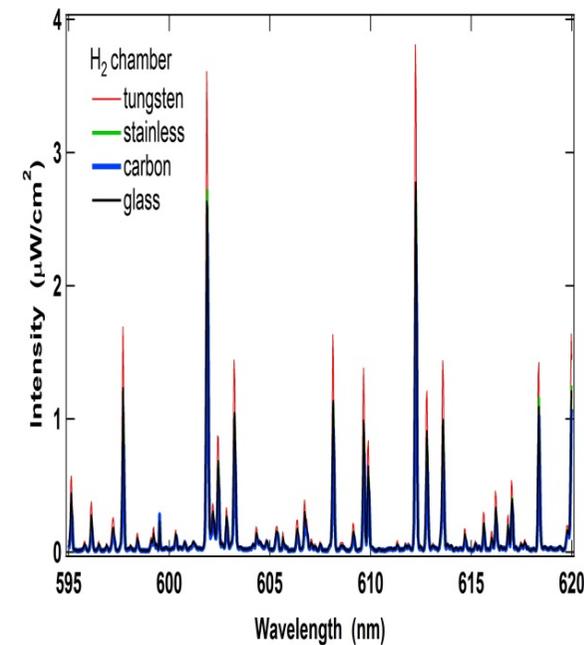
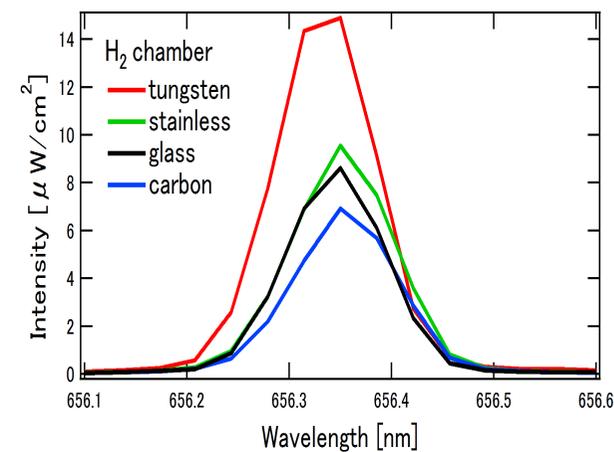


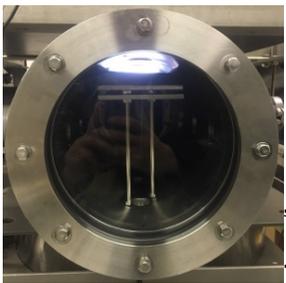
ガラス板



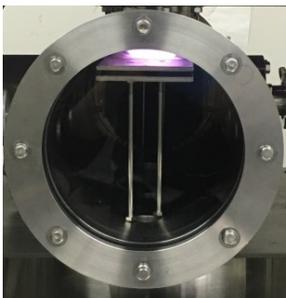
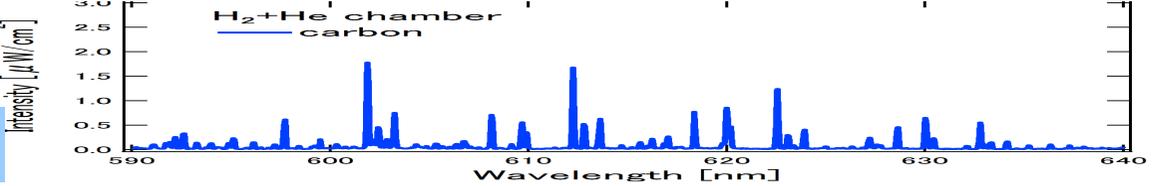
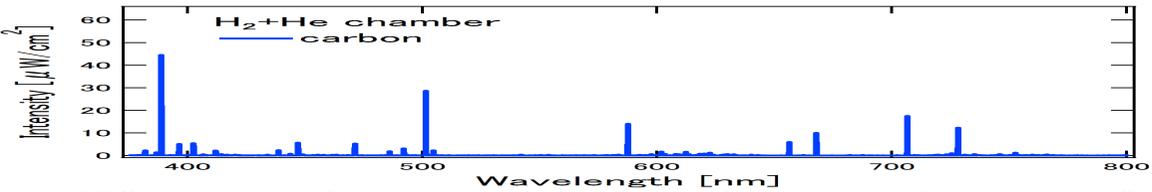
H₂ チャンバー部分 分光計測

H₂ 0.02 Torr
アンテナ出力1500 W

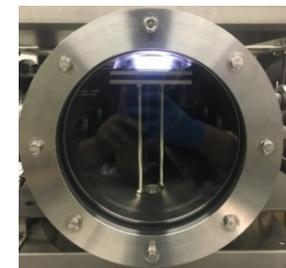
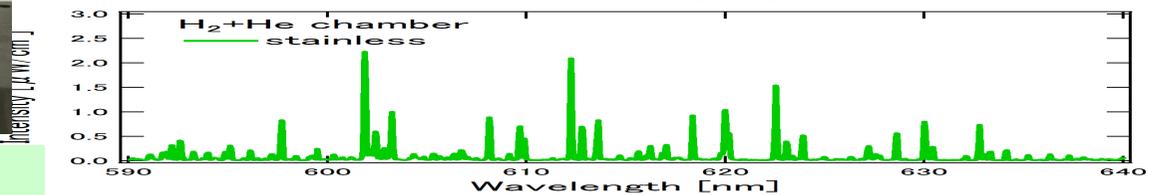
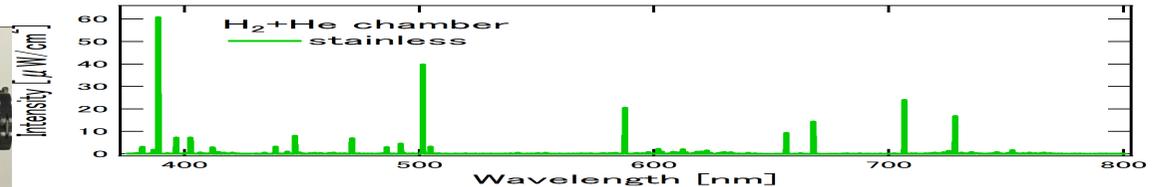




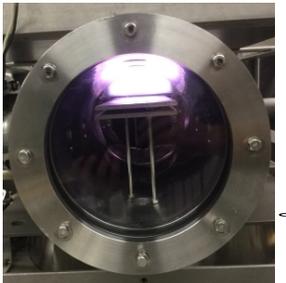
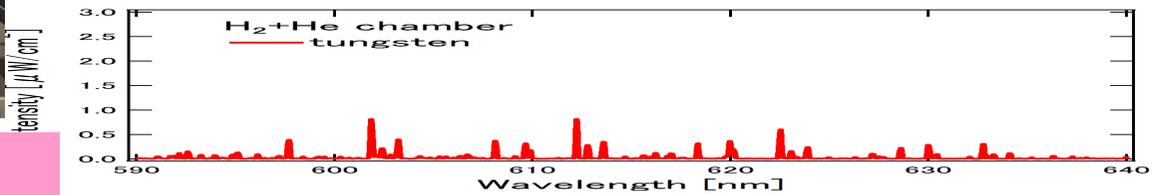
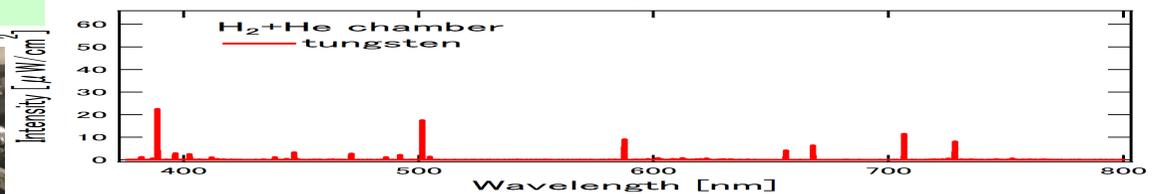
カーボン板



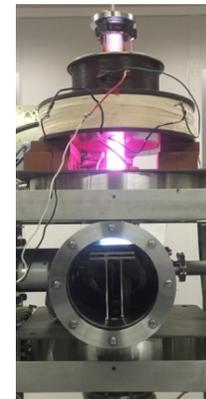
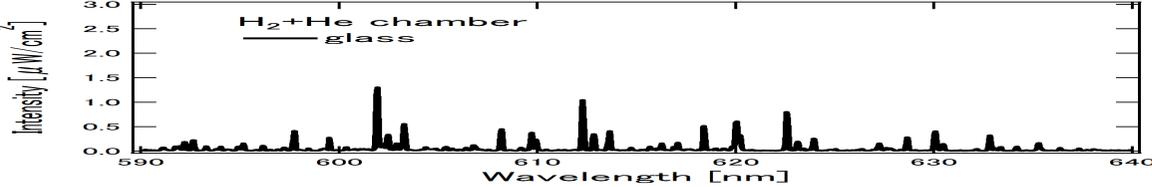
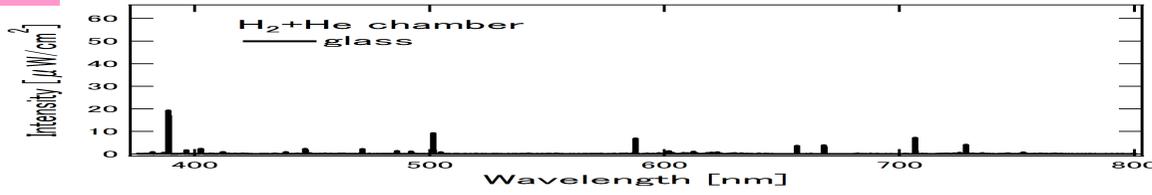
ステンレス板



タングステン板

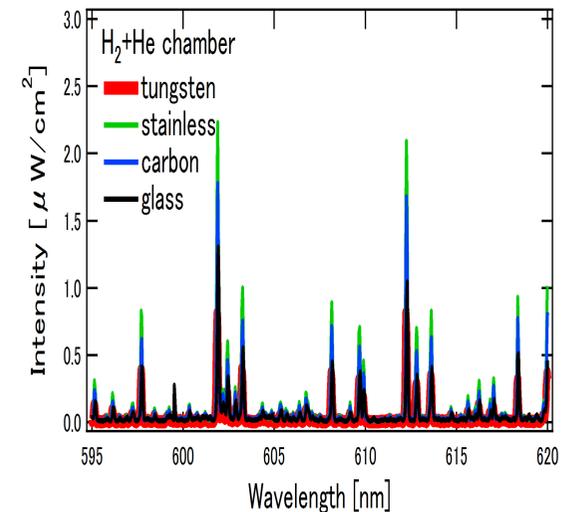
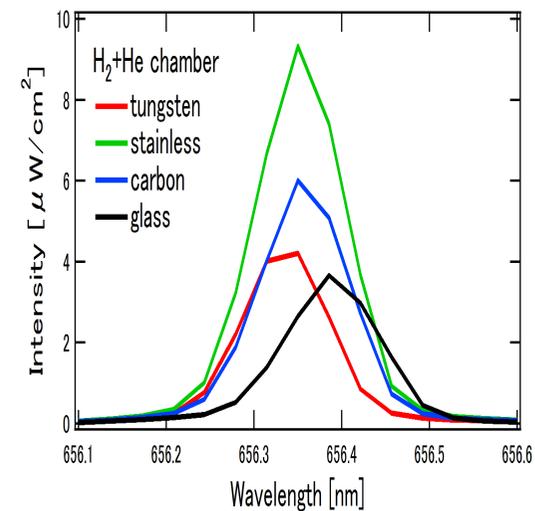


ガラス板

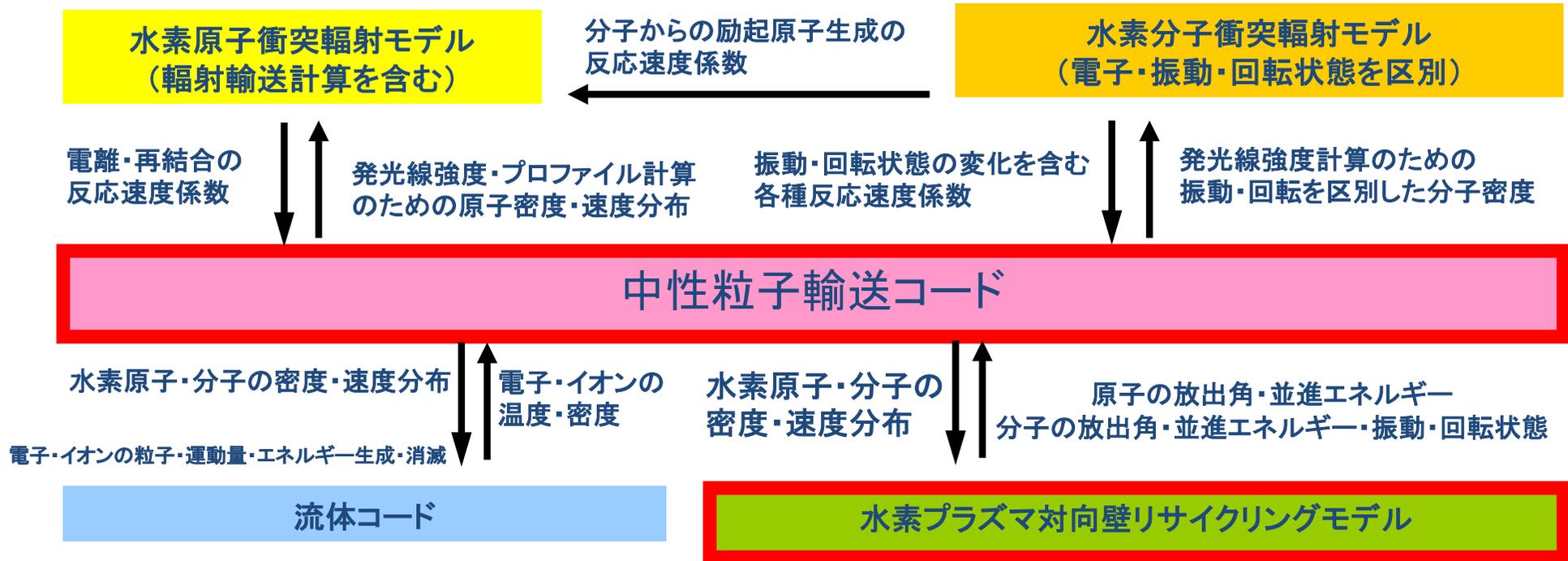


H₂+He チャンバー部 分光計測

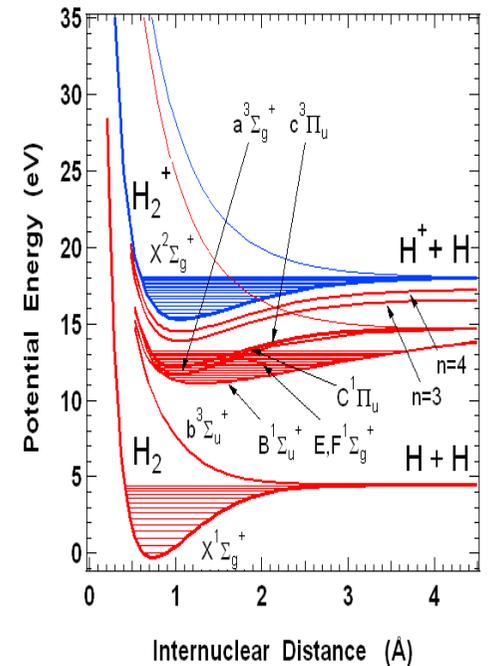
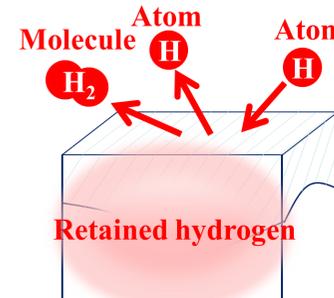
H₂ 0.01 Torr
He 0.04 Torr
アンテナ出力1500W

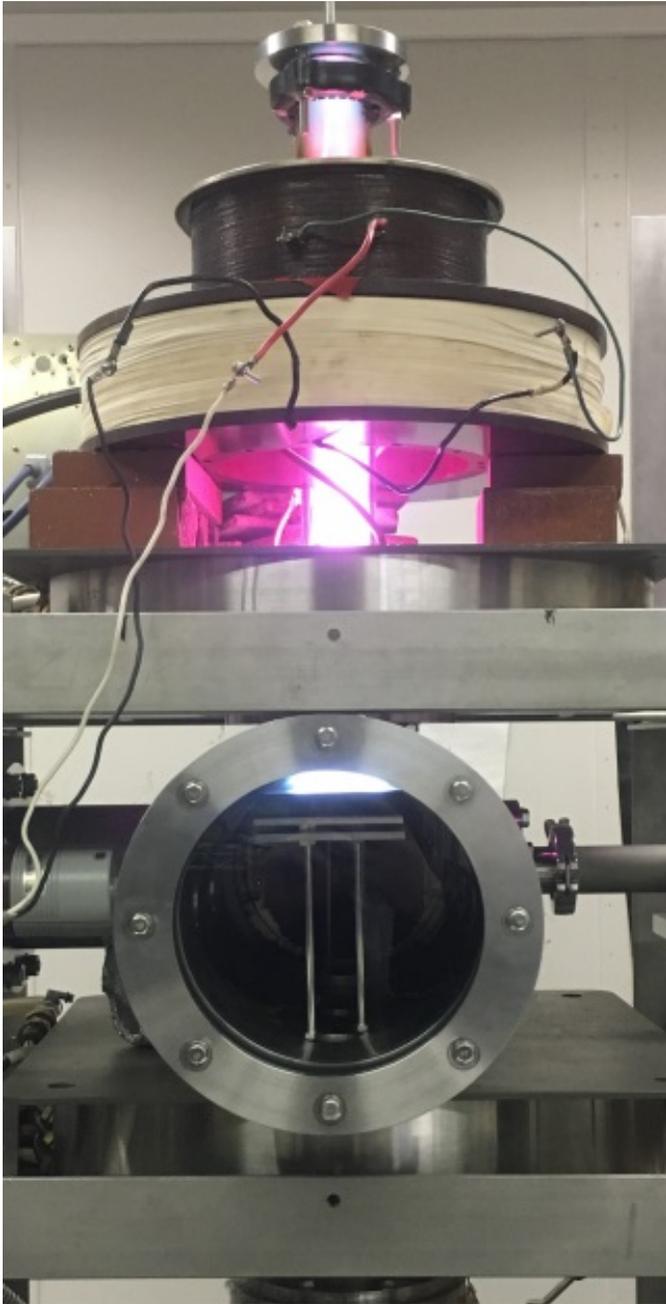


水素分子の電子・振動・回転状態を区別したコードの整備



- (1) ダイバータプラズマの水素分子との衝突によるエネルギー損失の計算 (H₂衝突輻射モデル)
- (2) H₂+H による水素原子のエネルギー損失 (中性粒子輸送コード: 信州大RFプラズマ)
- (3) いろいろな壁材における H の反射・再結合の実験
- (4) HD衝突輻射モデルの構築





HD分子 板で生成？

(ガラス管部での生成は小さい？)

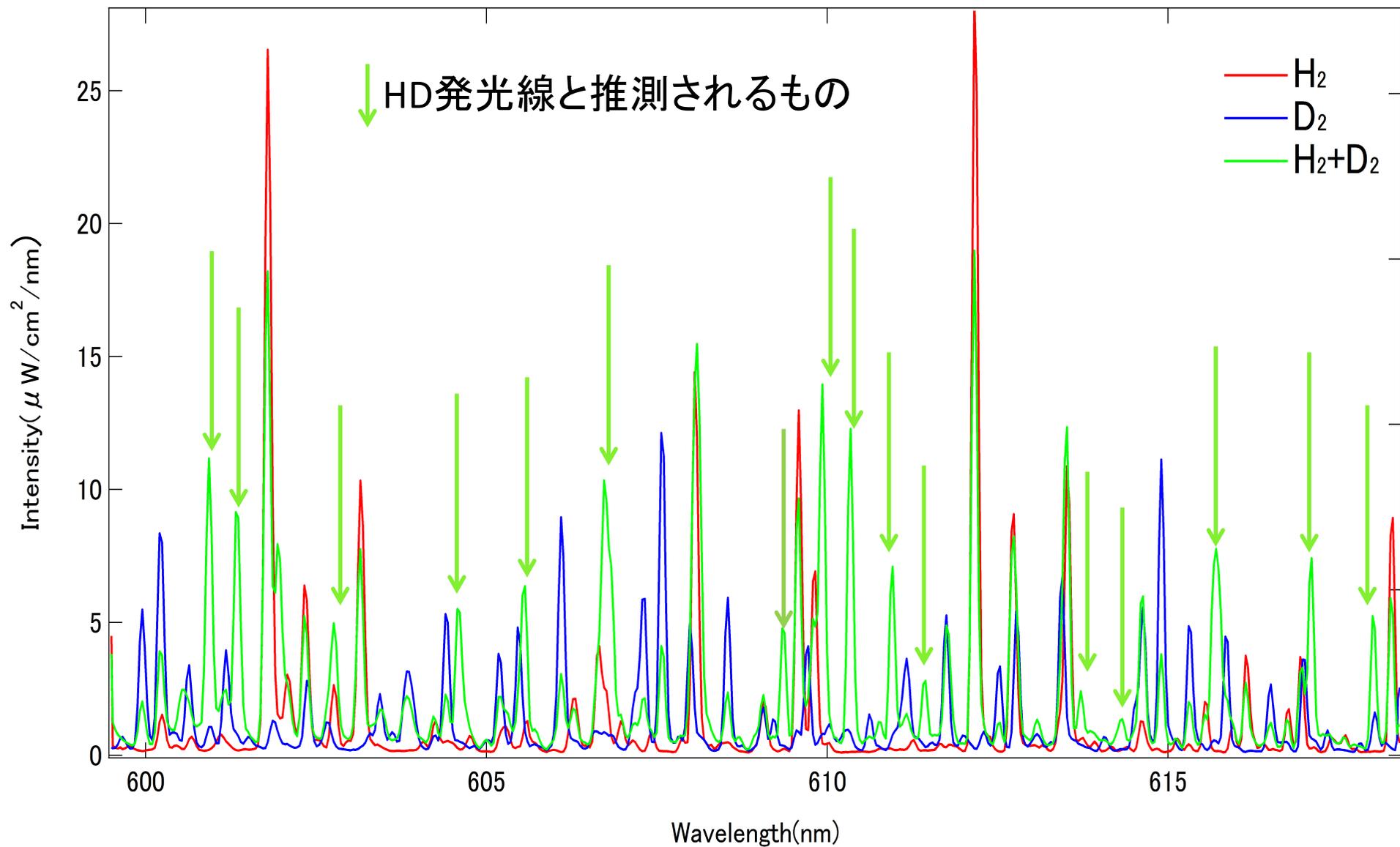
H₂:D₂:HD の密度比

板近傍の分子が板で生成されたものか、
入射ガス分子を見ているのかの指標になる。

全部板からなら

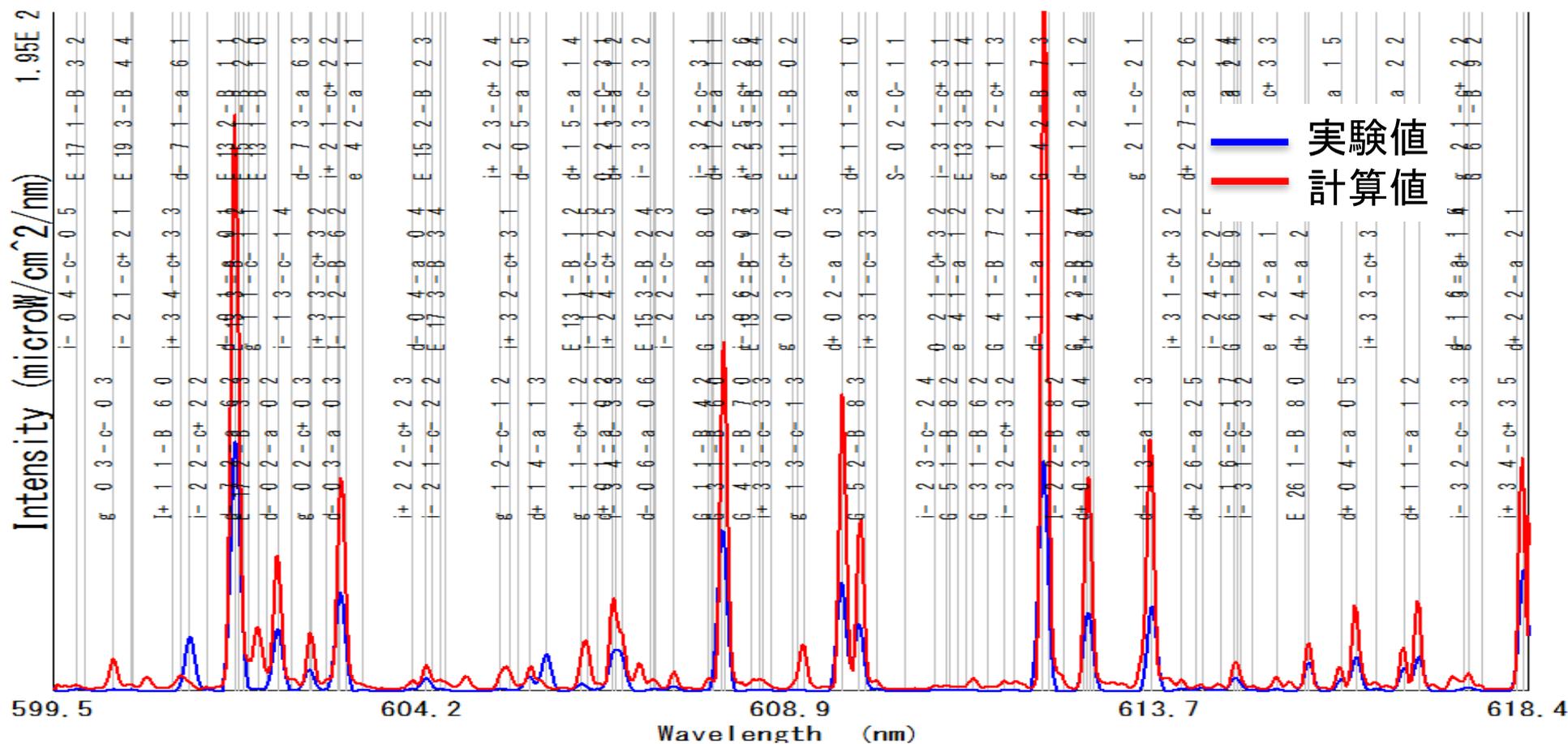
H₂:D₂:HD=1:1:2

H₂放電・D₂放電・H₂+D₂混合放電比較

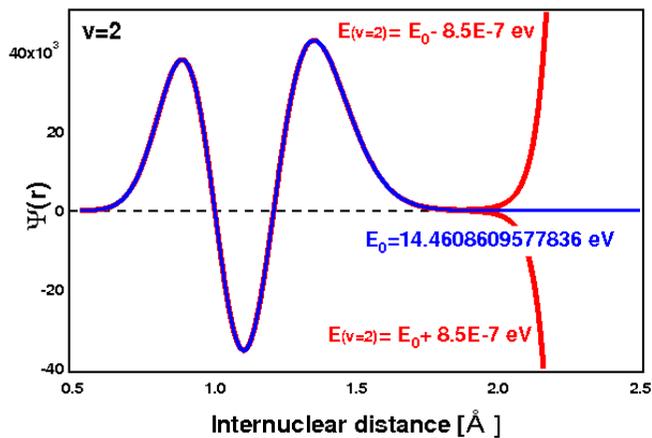


H₂波長による波長校正

H₂実験・計算比較32次



Energy level : Crosswhite, H.M. Hydrogen Molecule Wavelength Tables of Gerhard Heinrich Dieke; John Wiley & Sons Inc.: Hoboken, NJ, USA, 1972.

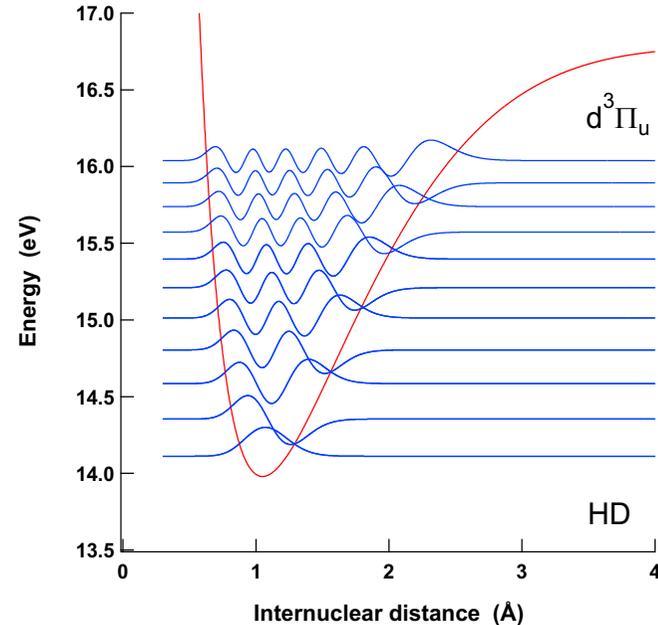
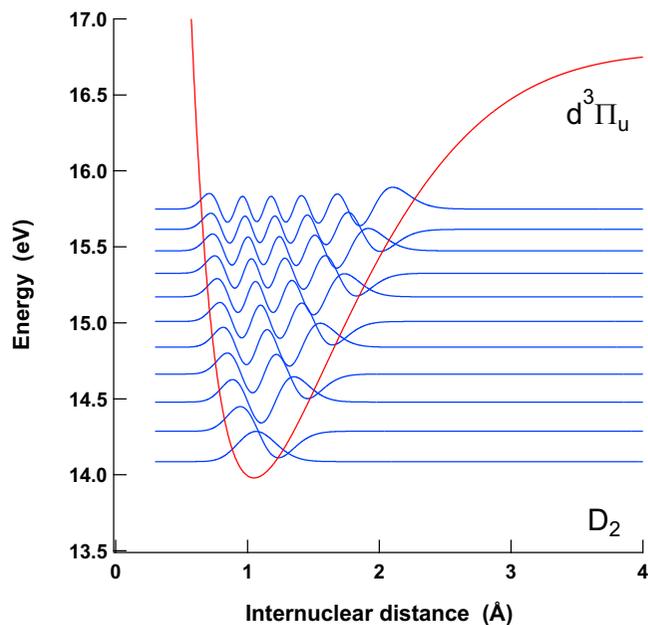
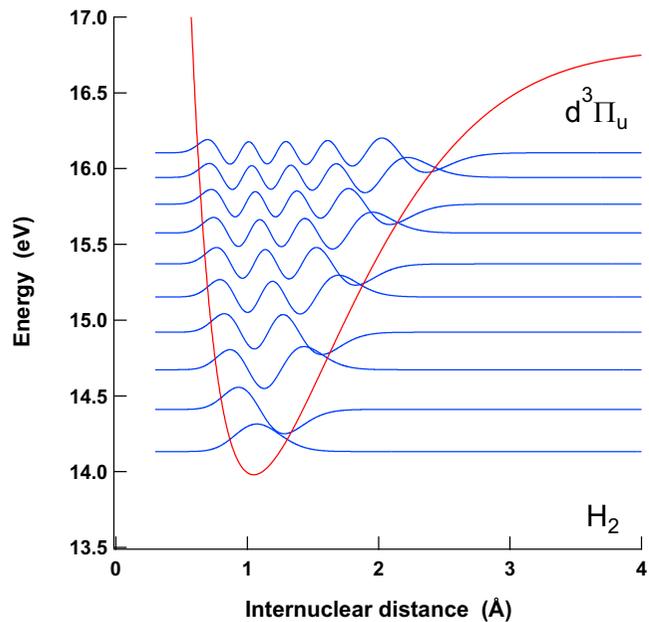


$$-\frac{\hbar^2}{2\mu} \frac{\partial^2 \psi_{nvJ}(R)}{\partial R^2} + \left(V(R) + \frac{\hbar^2 N(N+1)}{2\mu R^2} \right) \psi_{nvJ}(R) = E \psi_{nvJ}(R)$$

$R_{i+1} = R_i \pm h$ でTaylor展開

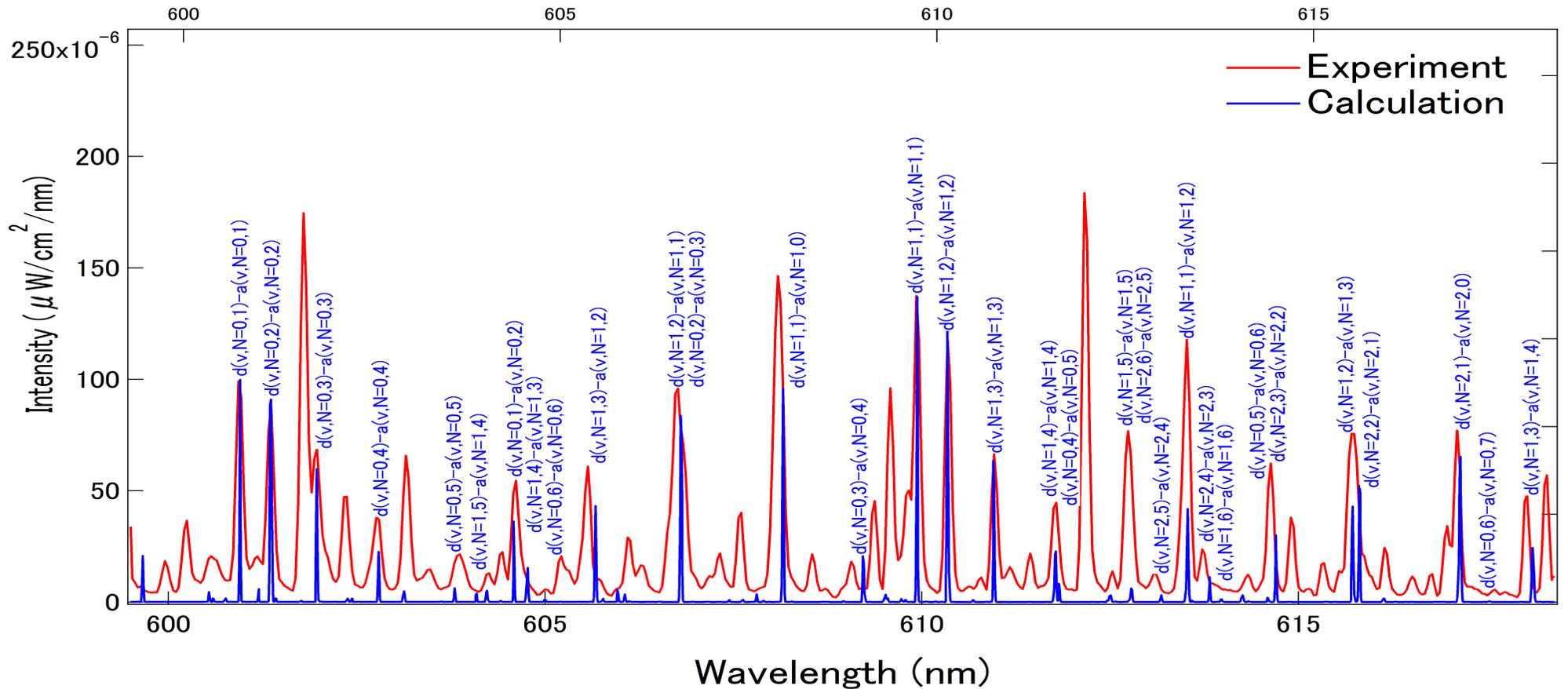
$$\left(1 + \frac{\hbar^2}{12} U(R_{i+1}) \right) \psi_{nvJ}(R_{i+1}) - 2 \left(1 - \frac{5\hbar^2}{12} U(R_i) \right) \psi_{nvJ}(R_i) + \left(1 + \frac{\hbar^2}{12} U(R_{i-1}) \right) \psi_{nvJ}(R_{i-1}) = 0$$

$$U(R) = \frac{2\mu}{\hbar^2} (E - V(R)) - \frac{N(N+1)}{R^2}$$



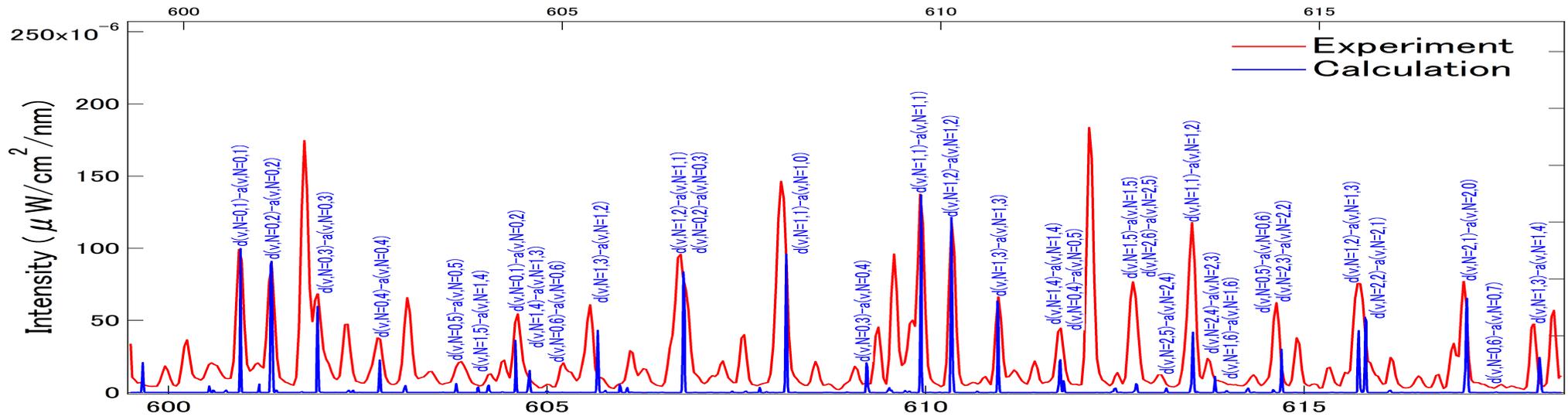
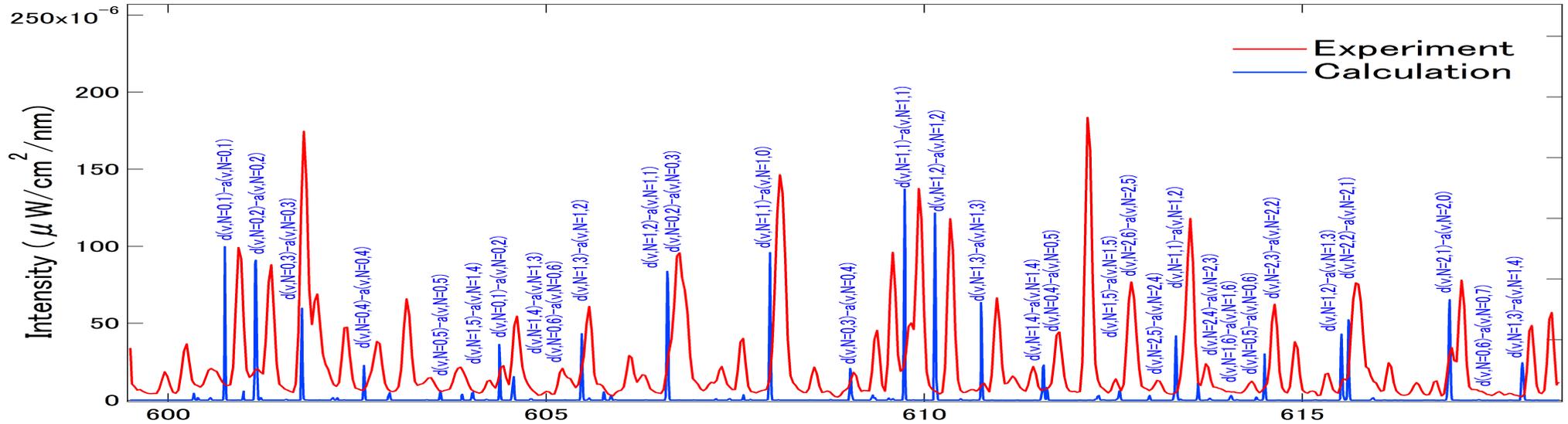
H₂+D₂ 放電

分光計測とHD分子衝突輻射モデル計算の比較



計算値を長波長側へ0.2[nm] 移動

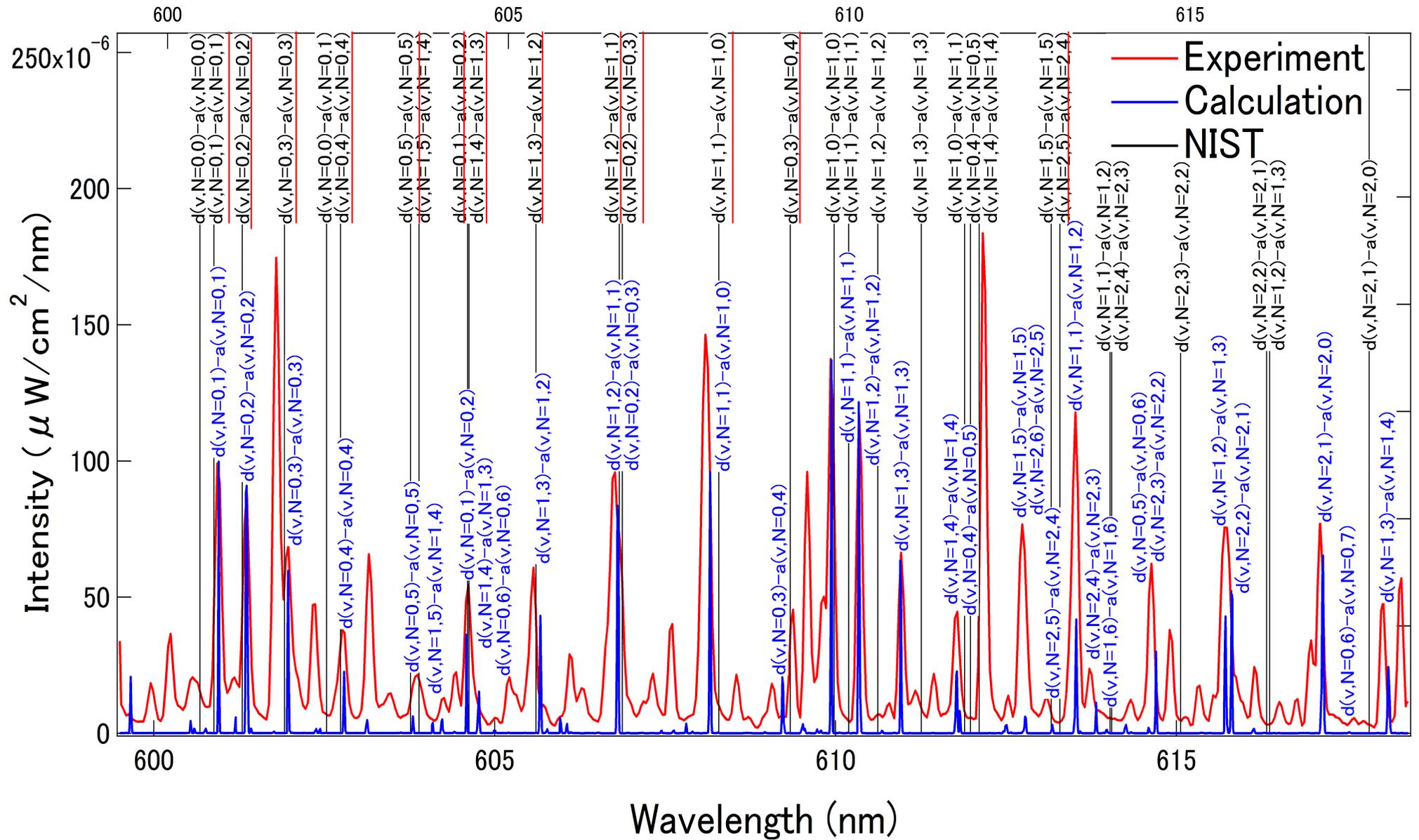
実験値・HD分子衝突輻射モデル計算値比較



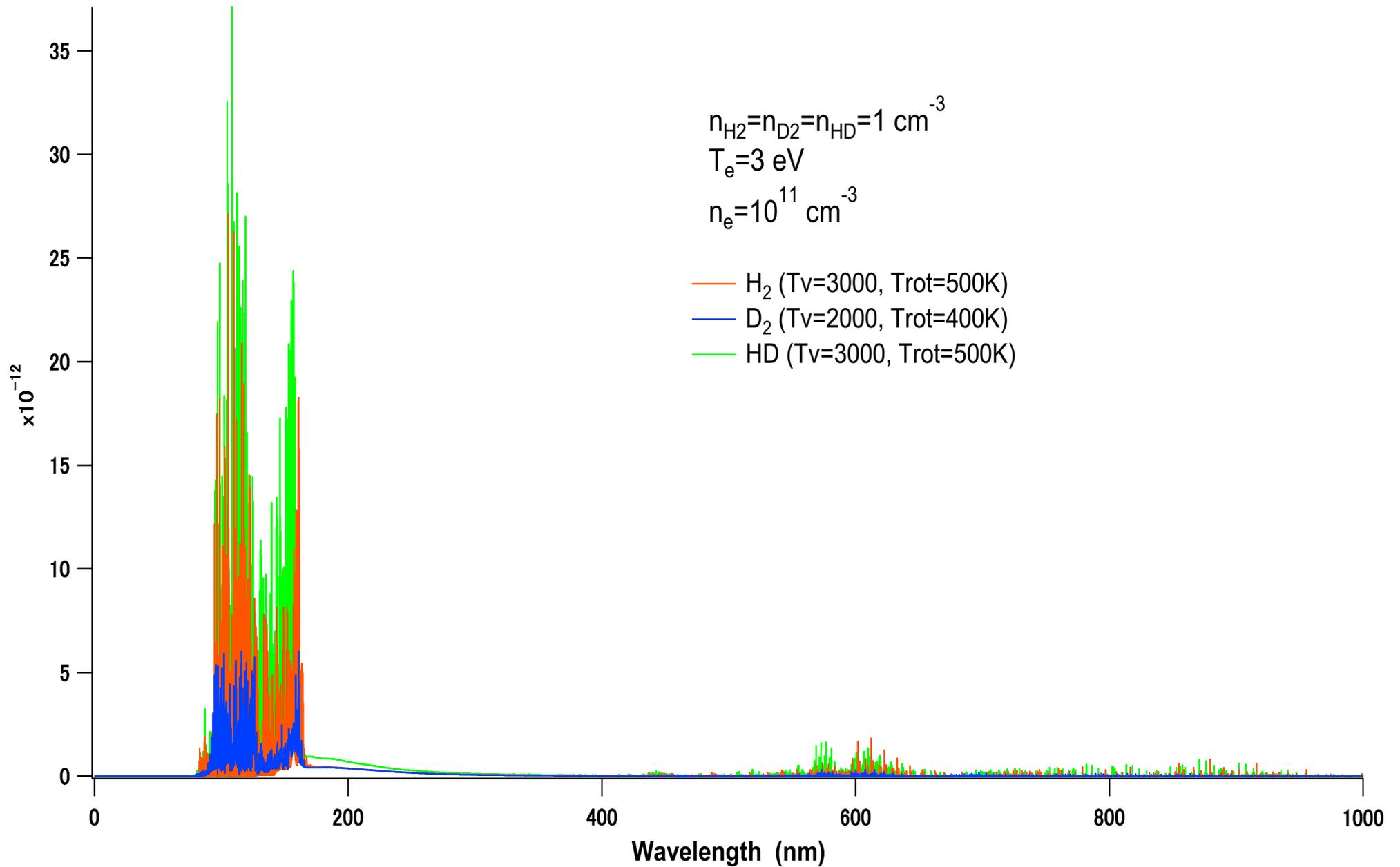
Wavelength (nm)

計算値を長波長側へ0.2[nm] 移動

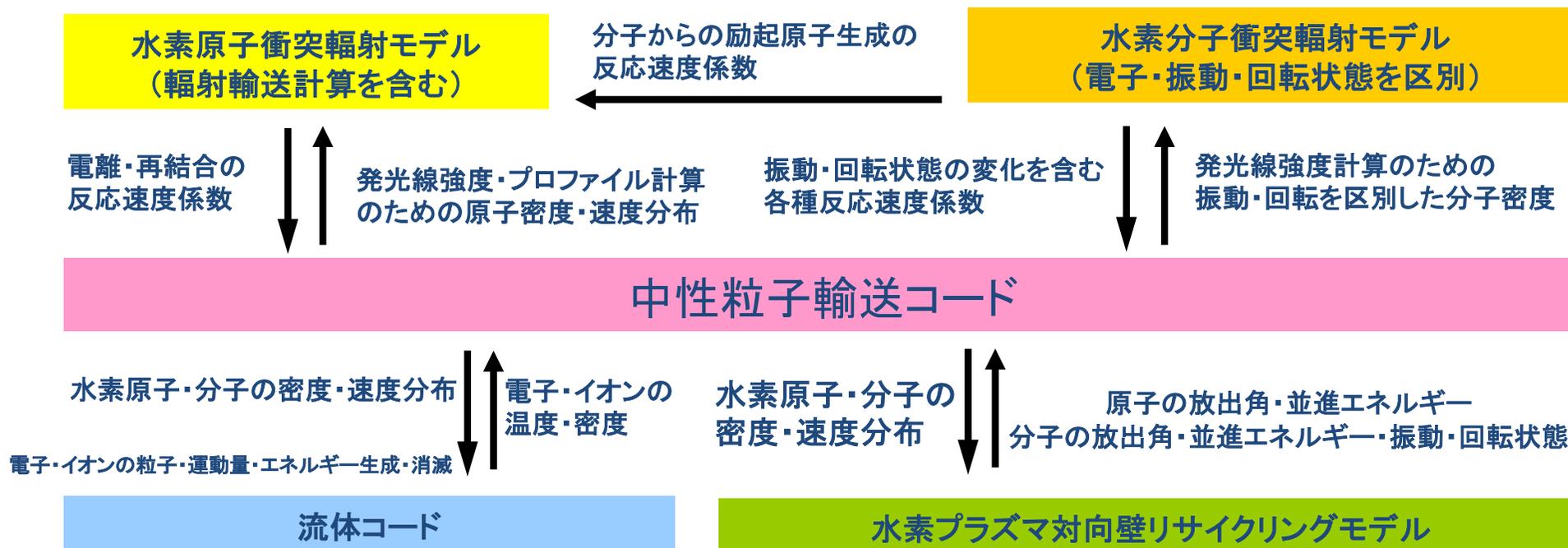
実験値・計算値比較



H₂ D₂ HD 発光線



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