Theoretical calculation on electron and molecular ion collisions relevant to divertor plasma

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Peculiar to molecule

- Vibrational and rotational freedom
- Dissociation, excited fragments
- Variety = State specific cross section
- Isotope effect

Needs of theoretical calculations

Molecular Assisted Recombination

- $\text{H}_2^+$ excited fragments $<$fuel$>$
- $\text{H}_3^+$ $<$dominant$>$
- $\text{CH}_n^+$ open shell $<$contamination$>$
- $\text{HeH}^+$ no crossing $<$product$>$

Their isotopes: D, T, $^{3,4}$He

Electron energy: 0.001—30eV $(1/E)$

NeH$^+$, He$_2^+$

Collision energy of electrons

- 1 eV

Rotational motion
Electronic excitation
Recombination
Indirect process

Bottleneck of Theoretical Calculation

Reliability: Over perturbation Theory
- Large scale calculation
  (partial waves, including states)

Applicability: Energy range
- Open shell electronic configuration
- Polyatomic molecules

Give a breakthrough to the bottleneck

Over perturbation theory /$\text{H}_2^+$

Ionic state: single-electron ex.
Dissociative state: two-electron ex.
Configuration Interaction V
Capture into Rydberg state
Non-adiabatic interaction

<Two-step method>
**Brief history of theory**

CI: Brdsley 1968, Resonance Theory  
Perturbation, Algebraic solution

NAI: Multichannel Quantum Defect Theory  
Seaton 1969, General formulation  
Fano 1970, Rotation  
Jungen Atabek 1977, Vibration  
Giusti 1980, Two-step method, DR

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**Scattering by the CI**

Lippman-Schwinger eqn. for K matrix

\[ K = V + V_G K \]

Perturbation (Born series): not converge generally  
Algebraic method: Chebyshev quadrature

\[ V_{rad} = C(R) \int V_{CI}(r) P_{CI}(r) \phi(r) dr \]

\[ V_{CI}(R) = \langle \phi_i(r;R) | H_{CI}(r;R) | \phi_i(r;R) \rangle R \]

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**CI as a function of R and E**

\[ V_{rad}(r) = \langle \phi_i(r;R) | H_{CI}(r;R) | \phi_i(r;R) \rangle R \]

Takagi, Hara, Sato 2009

H\(_2^+\) the lowest two-electron excited state

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**Low energy DR**

**Energies higher than 1 eV**

Descretized dissociative state  
E=0.3 --12 eV  
H\(_2^+\), D\(_2^+\), HD^+

Dissociative Recombination  
Dissociative Excitation  
for each vibrational state

Takagi 2002 Phys scripta

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**Hydrogen mol. at low energies**

Left problem: partial waves other than d\(\sigma\)  
1st. perturbation for the other:  
Data for D\(_2\), T\(_2\), DT could be easily obtained.

To increase reliability,  
We develop new method for a breakthrough.  
Main subject of us in this CRP

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**bottleneck**

First order other than the lowest diss. St.

Limited below 12 eV: only first excited state of ion core is included

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**2nd order improves?**

Fifiring & Store 2008

\[ \sum E \int dE_v \frac{\langle \psi_{E_v} | \hat{H} | \psi_{E_v} \rangle}{E_v - E} \]

Assume V (CI) is independent of E.

\[ V \] diverges logarithmically

Needs taking K diagonal elements

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**Non-crossing system/ HeH**

Takagi 1999, 2004: MQDT + discretized dissociative states

- Satisfy boundary condition of standing wave
- Not being understood?
- Show the reason of large cross section

Haxton & Greene 2009: MQDT + Siegert-pseudosatate

- Many partial waves

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**R-matrix calc. for QD**

Many partial waves

\[ \mathbf{R} \] matrix calculation for QD

Physics for large cross section

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**With experiment** Haxton & Greene

With experimental data

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**QD change and FC region**

Determine the cross sections

Common property in noble gas hydride ions

Florescu, Takagi, Mitchell (unpublished)

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**CRP**
Partial wave mixing

Takagi et al. 1991 for CH

\[ \sum_{N'N} N' \langle N' N | R \rangle \langle R | N N' \rangle \]

Takagi 2004 for HeH

\[ \sum_{N'N} N' \langle N' N | R \rangle \langle R | N N' \rangle \]

Curik, Greene 2007 for LiF

\[ \sum_{N'N} N' \langle N' N | R \rangle \langle R | N N' \rangle \]

Effect of mixing

no-mixing

no-mixing

no-mixing

CH\(+\), Takagi et al. 1991

HeH\(+\), Takagi 2004

LiH\(+\), Curik & Greene 2007

Small effect

About ten times

H\(_3^+\) major abundance

Greene’s group 2001: Jahn-Teller coupling

Jungen & Pratt 2009

\[ H (\rho, \phi) = \begin{pmatrix} W_0 + iN \rho^2 & f \rho e^{-i\phi} + g \rho^2 e^{2i\phi} \\ f \rho e^{i\phi} + g \rho^2 e^{-2i\phi} & W_0 + \frac{1}{2} \rho^2 \end{pmatrix} \]

Two-step method (traditional)

Non-adiabatic (present)

CRP: dissociation /LS eq.

MQDT: vibronic

CRP with dissociation

“strong non-adiabatic coupling representation”

Collision energy of electrons

1 eV

Rotational motion

Electronic excitation

Recombination

Indirect process

MQDT Frame Transform.

Hertzberg-Teller expansion

Adiabatic approximation in electron scattering

Energy & R

H\(_2\) (crossing exists)

K\(_E\)(R)
MQDT with dissociation

Discretization of dissociative states

\[ \chi_R^{(A)} = \frac{1}{\sqrt{\Delta_\text{R}}} \int_{R_{\text{min}}^{(A)}}^{R_{\text{max}}^{(A)}} \chi_R^{(A)}(\bar{R}) d\bar{R} \]

Normalization: state (non-observed ch.)/energy (observed ch.) could change

For avoid singularity

Finite, non-singular

Boundary condition/Normalization

\[ \Psi^{(A)}(r_a, R) = \sum_q C_q \phi_q(r_a) \chi_q(R) \]

MQDT outer region

\[ \Psi^{(A)}(r_a, R) \to \sum_{L=0}^{\infty} \delta_{L,0} \phi_{L,0}(r_a) \chi_{L,0}(R) + K_{L,0}^{(A)}(r_a) \chi_{L,0}(R) \cos(kR) \]

All R region

\[ K_{L,0}^{(A)} = \Delta_{L,0}^{-1/2} \nu_{L,0}^{3/2} K_{L,0}^{(A)} \]

Asymptotic wave function

An asymptotic wave function gives information on the final channels: each state and energy

Advantage over Siegert-pseudostate method

R-matrix calculation

Collaborator

Motomichi Tashiro (Institute for Molecualr Science)

UK R-matrix program

Now testing the present approach for HeH

Detail of quantum defect

Including partial wave mixing

HeH

Haxton & Greene

Takagi 2004

Tashiro (proceeding)

DVR method for tri-atomic dissociative states

Collaborator

Kazuhiro Sakimoto (Japan Aerospace Exploration Agency)

Our aim

Wide energy range (1meV—30eV)

Reliable and

For various (highly excited) rotation-vibration states
Plan for CRP

(1) CS by accurate CI for $D_2$, $T_2$, TD
   (H$_2$ was finished 2008, JAEA, Sawada)
   <finish in 2009>

(2) Over perturbation for every excited channels by R-matrix calc. for adiabatic electro. st. (HeH, H$_2$, NeH)

(3) Calc. by strong non-adiabatic coupling representation (H$_2$, CH)
   <partially obtain result in 2009>

(4) calc. on H$_3^*$
   <start 2009>