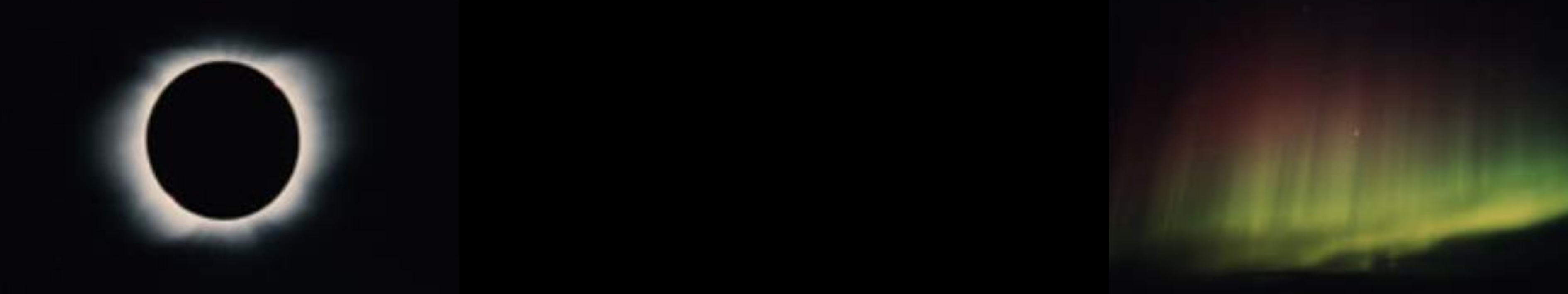
アテナシス（Athenasys Co., Ltd）のご紹介



会社紹介

https://athenasys.co.jp/

設立：2008年 10月 1日

事業内容：ライセンス販売（一部，サポート・コンサルティング）

取り扱っている製品

BOSPROM：プラズマシミュレーションで用いる輸送係数・反応レートの計算ツール（自社製品）

Lennard-Jones パラメータ 推算ツール（自社製品）

パートナー会社：Quantemol（英国）　※アテナシスは日本国内の代理店

Quantemol-VT（QVT）：HPEM を core としたプラズマシミュレーションソフトウェア

Quantemol-DB（QDB）：反応データベース，Global Model（QGM）

Quantemol-EC（QEC）：分子に対する電子衝突断面積の計算ツール

重点分野：

半導体製造装置のプラズマプロセス

その他，低温非平衡プラズマプロセス，電子衝突断面積を必要とする反応プロセス

主要なお客様：

半導体製造装置メーカー，デバイスメーカー

担当者はアネルバ（現キヤノンアネルバ）で半導体製造装置の研究開発に長年従事

会社紹介 (2)

参加している学会，委員会

応用物理学会　：個人会員

DXプラズマプロセス委員会：企業会員

IOP (Institute of Physics) ：個人会員

化学工学会　　：CVD反応分科会の個人会員

電気学会　　　：液界面プラズマの実験・計算モデル標準化調査専門委員会

原子・分子衝突断面積および放電基礎データ査専門委員会

放電・プラズマ気相シミュレーション技法調査専門委員会

結晶成長学会　：個人会員（休眠中）

153委員会　　：終了後，DXプラズマプロセス委員会へ

参加している NPO

原子分子データ応用フォーラム

Swarm パラメータ，反応レートの Lookup Table 作成ツール

BOSPROM

プロパゲータ法 (分布関数 $f(\vec{v})$ 計算法の一種)

流体モデル

$n_e(\vec{r}, t)$
$T_e(\vec{r}, t)$

CFD-ACE+など

近似：Maxwell分布

Boltzmann eq. $\boldsymbol{f(\vec{r}, \vec{v}, t)}$

近似：位置空間一様

簡略化Boltzmann eq.

$$\frac{\partial}{\partial t} f(v, \theta, t) = \left[-a \frac{\partial}{\partial v_x} + \left(\frac{\partial}{\partial t} \right)_{\text{coll}} \right] f(v, \theta, t)$$

二項近似

BOLSIG+, CFD-ACEなど

近似： $f \propto F_0(\varepsilon) + F_1(\varepsilon) \cos\theta$

確率的解法

Monte-Carlo法

MagBoltzなど

直接解法

プロパゲータ法

BOSPROM
(**Bo**ltzmann **S**olver by **Pro**pagator **M**ethod)

衝突断面積 → 分布関数 f → 反応レート定数, 輸送係数(移動度, 拡散係数)

Swarm parameters

BOSPROM:衝突断面積データ選択・編集画面

- 断面積データの編集が可能

D:/tukasa/home/bosprom/Ar_hu_13M_.atp

File Edit Graph Prefer Help

σ | Setup | Results | LUT

Library

Ar	EFFECTIVE
Ar -> Ar*(11.5eV)	EXCITATIC
Ar -> Ar^+	IONIZATIC
CH4 -> CH3+H^-	ATTACHMEN
CH4 -> H2+CH2^-	ATTACHMEN
CH4	ELASTIC
CH4 -> CH4(V24)(0.162eV)	EXCITATIC
CH4 -> CH4(V13)(0.361eV)	EXCITATIC
CH4 -> CH4*(9eV-dissoc)	EXCITATIC
CH4 -> CH4*(10eV-dissoc)	EXCITATIC
CH4 -> CH4*(11eV-dissoc)	EXCITATIC
CH4 -> CH4*(12eV-dissoc)	EXCITATIC
CH4 -> CH4^+	IONIZATIC
CH4 -> H+CH3^+	IONIZATIC
CF4 -> CF2^-+F2	ATTACHMEN
CF4	ELASTIC
CF4 -> CF4(V24)(0.08eV)	EXCITATIC
CF4 -> CF4(V13)(0.166eV)	EXCITATIC
CF4 -> CF4*(7.57eV)	EXCITATIC
CF4 -> CF2+F2(12.7eV)	EXCITATIC
CF4 -> CF4^+	IONIZATIC
Cl2 -> Cl^- + Cl	ATTACHMEN
Cl2	ELASTIC
Cl2 -> Cl2(v1)	EXCITATIC
Cl2 -> Cl2(v2)	EXCITATIC

All Registered

01	Ar	EFFECTIVE	1.3
02	Ar -> Ar*(11.5eV)	EXCITATION	11.
03	Ar -> Ar^+	IONIZATION	15.

Gnuplot (window id : 0)

Dialog

Name

Ar -> Ar*(12.9eV)

Collision Type

EXCITATION

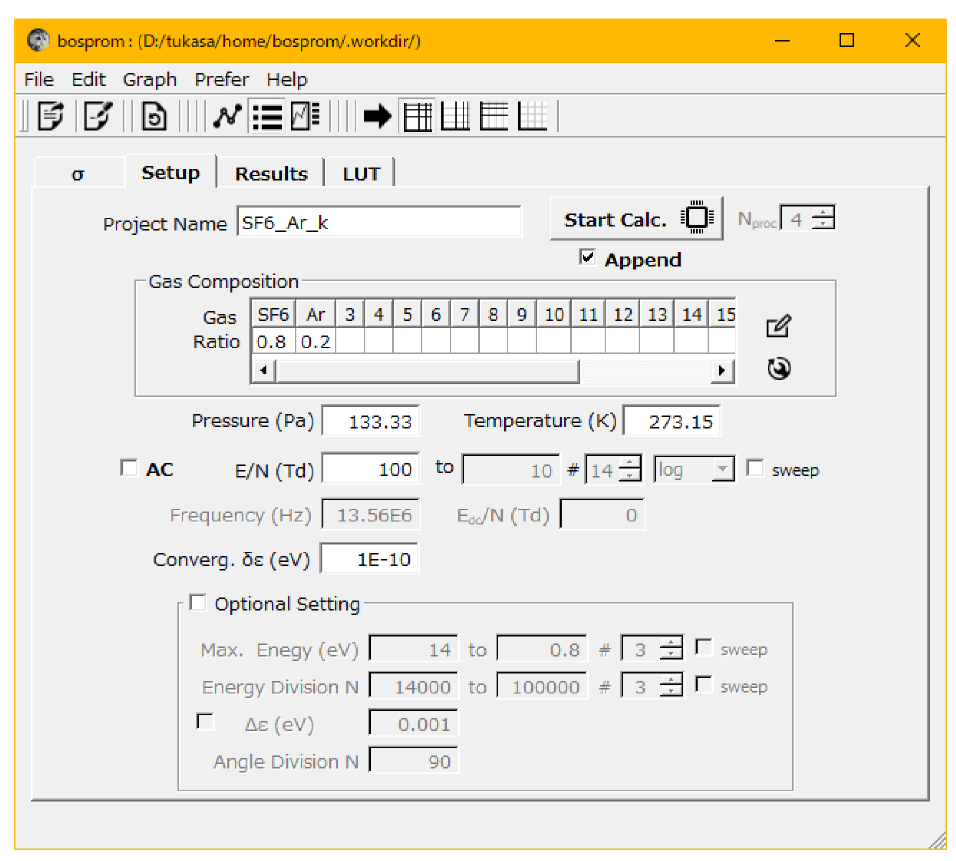
Threshold (eV) or Mass Ratio

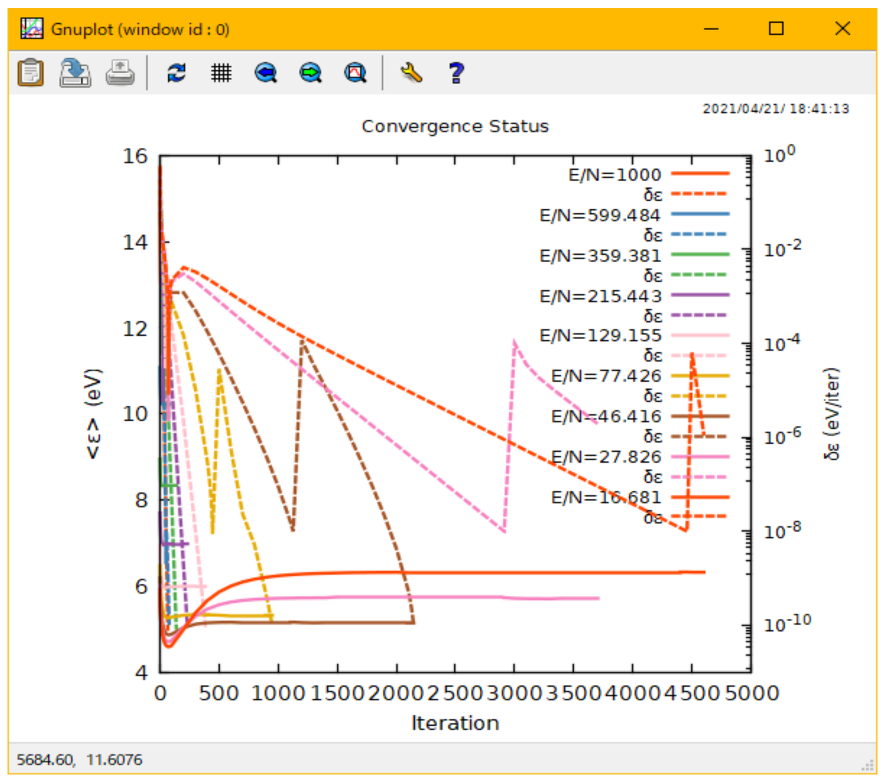
12.900

	X Data	Y Data
1	0.05	0
2	12.9	0
3	12.95	0.0495
4	13	0.08
5	13.05	0.0915
6	13.1	0.084
7	13.15	0.086
8	13.2	0.088
9	13.25	0.09
10	13.3	0.092
11	13.35	0.094
12	13.4	0.096
13	13.45	0.098
14	13.5	0.1
15	13.55	0.1015
16	13.6	0.103
17	13.65	0.1045
18	13.7	0.106
19	13.75	0.1075

Delete | Insert Before | Append Last | OK | Cancel

BOSPROM:計算条件設定画面・収束状況表示





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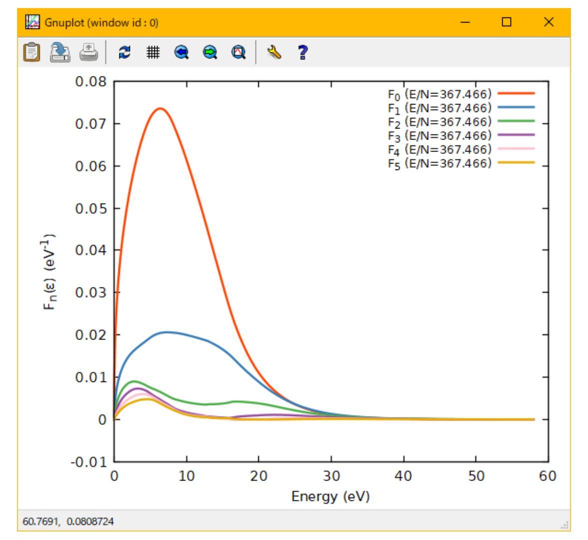
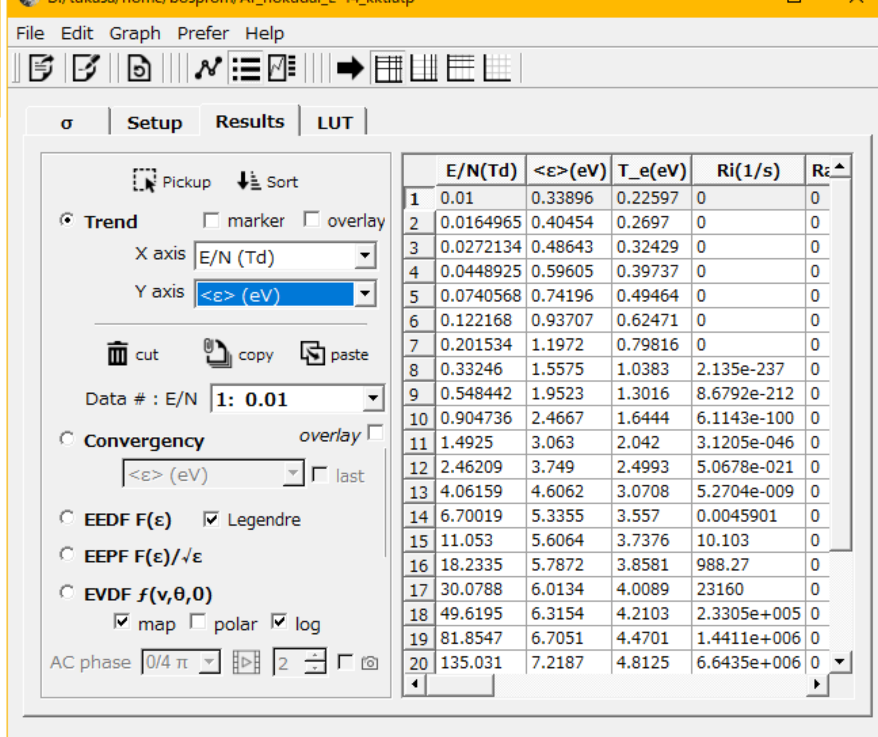
BOSPROM：結果表示画面





	E/N(Td)	<ε>(eV)	T_e(eV)	Ri(1/s)	Ra
1	0.01	0.33896	0.22597	0	0
2	0.0164965	0.40454	0.2697	0	0
3	0.0272134	0.48643	0.32429	0	0
4	0.0448925	0.59605	0.39737	0	0
5	0.0740568	0.74196	0.49464	0	0
6	0.122168	0.93707	0.62471	0	0
7	0.201534	1.1972	0.79816	0	0
8	0.33246	1.5575	1.0383	2.135e-237	0
9	0.548442	1.9523	1.3016	8.6792e-212	0
10	0.904736	2.4667	1.6444	6.1143e-100	0
11	1.4925	3.063	2.042	3.1205e-046	0
12	2.46209	3.749	2.4993	5.0678e-021	0
13	4.06159	4.6062	3.0708	5.2704e-009	0
14	6.70019	5.3355	3.557	0.0045901	0
15	11.053	5.6064	3.7376	10.103	0
16	18.2335	5.7872	3.8581	988.27	0
17	30.0788	6.0134	4.0089	23160	0
18	49.6195	6.3154	4.2103	2.3305e+005	0
19	81.8547	6.7051	4.4701	1.4411e+006	0
20	135.031	7.2187	4.8125	6.6435e+006	0

ATHENASYS

BOSPROM:プラズマ計算用 lookup-table 作成画面

bosprom : (D:/tukasa/home/bosprom/.workdir/)

File Edit Graph Prefer Help

σ | Setup | Results | LUT

Update D=μT_e

Number of data 120

Pressure (Pa) 13.333

k order 4 2 3 1

T_e range 2 50

N_e (m^{-3}) 1E+13

Y-axis k1 (m^3/s)

marker overlay

Export (CFD-ACE+)

Te - k, μ, D   Te - k

R_name Argon_hokudai

Import CFD-ACE+

Equally spaced

	Te (eV)	k1 (m^3/s)	k2 (m^3/s)	k3 (m^3/s)
1	2	0	2.47996e-24	2.65474e-25
2	2.40336	0	6.79372e-24	7.27252e-25
3	2.80672	1.83832e-27	7.63325e-20	1.23452e-19
4	3.21008	3.84433e-27	1.5962e-19	2.58164e-19
5	3.61345	2.94471e-21	1.56789e-18	4.68609e-18
6	4.01681	3.5004e-18	3.0896e-17	4.74729e-17
7	4.42017	7.78969e-17	2.08562e-16	1.72251e-16
8	4.82353	4.07528e-16	5.53056e-16	3.85831e-16
9	5.22689	1.05326e-15	9.51372e-16	6.73392e-16
10	5.63025	1.96409e-15	1.36599e-15	1.01721e-15
11	6.03361	2.94441e-15	1.76166e-15	1.36413e-15
12	6.43697	4.30907e-15	2.05253e-15	1.7282e-15
13	6.84034	5.67374e-15	2.3434e-15	2.09227e-15
14	7.2437	7.0384e-15	2.63427e-15	2.45634e-15
15	7.64706	8.40306e-15	2.92514e-15	2.82042e-15
16	8.05042	9.77468e-15	3.19317e-15	3.16977e-15
17	8.45378	1.11806e-14	3.34845e-15	3.44651e-15
18	8.85714	1.25865e-14	3.50372e-15	3.72325e-15
19	9.2605	1.39924e-14	3.659e-15	3.99999e-15
20	9.66387	1.53983e-14	3.81428e-15	4.27673e-15

- 計算結果から T_e ベースの LUT (lookup-table) を作成
- CFD-ACE+ や COMSOL に import する format で出力が可能

Lennard-Jones パラメータ推算ツール

分子の加算因子・沸点から Lennard-Jones パラメータを推算

熱流体・プラズマのシミュレーションで必要となる L-J parameters を推算

表２－１　Lyndersenの臨界定数の加算因子

	個数
非環状加算因子	
-CH3	1
-CH2-	0
>CH-	0
>C<	0
=CH2	0
=CH-	0
=C<	0
=C=	0
#CH	0
#C-	0
環状加算因子	
-CH2-(R)	0
>CH-(R)	0
>C<(R)	0
=CH-(R)	6
=C<(R)	0
=C=(R)	0

	個数
ハロゲン加算因子	
-F	5
-Cl	0
-Br	0
-I	0
酸素加算因子	
-OH(Alcohol)	0
-OH(Phenol)	0
-O-	0
-O-(R)	0
>C=O	0
>C=O(R)	0
O=HC-(Aldehyde)	0
-COOH(Acid)	0
-COO-(Ester)	0
=O	0

	個数
窒素加算因子	
-NH2	0
>NH	0
>NH(R)	0
>N-	0
>N-(R)	0
-CN	0
-NO2	0
イオウ加算因子	
-SH	0
-S-	0
-S-(R)	0
=S	0
その他	0
>Si<	0
>B-	0

Lyndersenの方法		
標準沸点Tb(K):	390.65	(Input)
分子量（M）：	182.10	(Input)
偏心因子ω	0.51	
Tc	548.65	
Pc	26.71	
Vc	401.00	
Lennard-Jones		
σ	6.33	
ε/k	481.79	(K)

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プラズマシミュレーション
ソフトウェア
QVT（HPEM）

Hybrid Plasma Equipment Model (HPEM)

IOP PUBLISHING JOURNAL OF PHYSICS D: APPLIED PHYSICS

J. Phys. D: Appl. Phys. 42 (2009) 194013 (20pp) doi:10.1088/0022-3727/42/19/194013

REVIEW ARTICLE

※ HPEM に GUI を追加したものが Q-VT

Hybrid modelling of low temperature plasmas for fundamental investigations and equipment design

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Received 12 May 2009, in final form 12 June 2009
Published 18 September 2009
Online at stacks.iop.org/JPhysD/42/194013

Abstract
The modelling of low temperature plasmas for fundamental investigations and equipment design is challenged by conflicting goals—having detailed, specialized algorithms which address sometimes subtle physical phenomena while also being flexible enough to address a wide range of process conditions. Hybrid modelling (HM) is a technique which provides many opportunities to address both fundamental physics and practical matters of equipment design. HM is a hierarchical approach in which modules addressing different physical processes on vastly disparate timescales are iteratively combined using time-slicing techniques. By compartmentalizing the physics in each module to accept given inputs and produce required outputs, different algorithms can be used to represent the same physical processes. In this manner, the algorithms best suited for the conditions of interest can be used without affecting other modules. In this paper, the basis and implementation of HM are discussed using examples from simulations of inductively coupled plasmas.

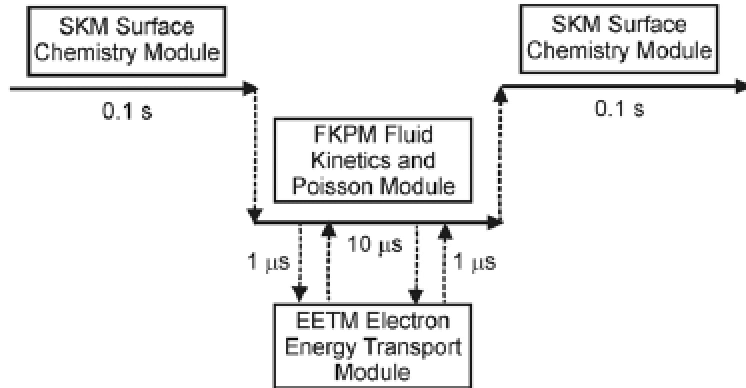

Figure 4. Schematic of time slicing between modules where the final outcome is a SS solution. Sub-time slicing may occur between the FKPM and EETM as those modules are more tightly coupled.

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HPEM の計算例

※ ミシガン大と Samsung の共著

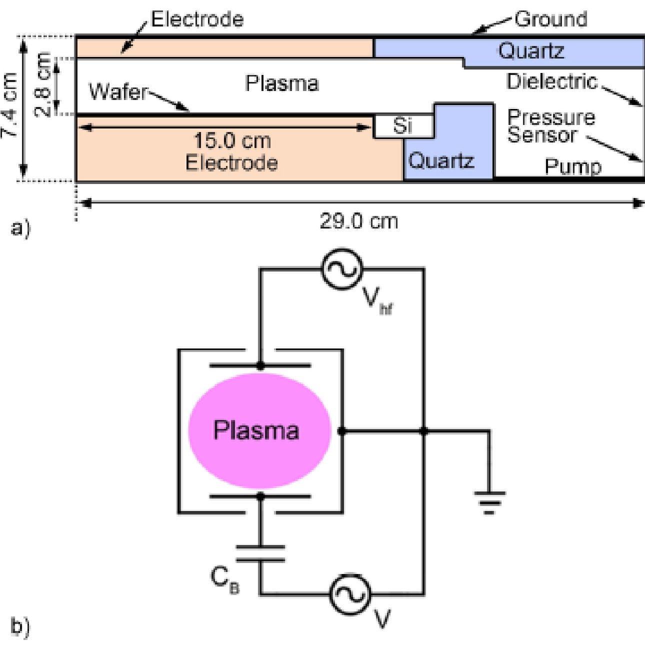

FIG. 1. Schematics of the reactor. (a) The two frequency CCP has the VWT power applied to the lower electrode and a sinusoidal, 80 MHz waveform applied to the top. (b) Electrical schematic of the system. Reproduced with permission from Kruger *et al.*, Plasma Sources Sci. Technol. **30**, 085002 (2021). Copyright 2021 IOP Publishing Ltd.

Voltage waveform tailoring for high aspect ratio plasma etching of SiO_2 using $Ar/CF_4/O_2$ mixtures: Consequences of ion and electron distributions on etch profiles

Cite as: J. Vac. Sci. Technol. A 41, 013006 (2023); doi: 10.1116/6.0002290
Submitted: 14 October 2022 · Accepted: 13 December 2022 ·
Published Online: 30 December 2022

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ABSTRACT

The quality of high aspect ratio (HAR) features etched into dielectrics for microelectronics fabrication using halogen containing low temperature plasmas strongly depends on the energy and angular distribution of the incident ions (IEAD) onto the wafer, as well as potentially that of the electrons (EEAD). Positive ions, accelerated to high energies by the sheath electric field, have narrow angular spreads and can penetrate deeply into HAR features. Electrons typically arrive at the wafer with nearly thermal energy and isotropic angular distributions and so do not directly penetrate deeply into features. These differences can lead to positive charging of the insides of the features that can slow etching rates and produce geometric defects such as twisting. In this work, we computationally investigated the plasma etching of HAR features into SiO_2 using tailored voltage waveforms in a geometrically asymmetric capacitively coupled plasma sustained in an $Ar/CF_4/O_2$ mixture at 40 mTorr. The tailored waveform consisted of a sinusoidal wave and its higher harmonics with a fundamental frequency of 1 MHz. We found that some degree of control of the IEADs and EEADs is possible by adjusting the phase of higher harmonics φ through the resulting generation of electrical asymmetry and electric field reversal. However, the IEADs and EEADs cannot easily be separately controlled. The control of IEADs and EEADs is inherently linked. The highest quality feature was obtained with a phase angle $\varphi = 0°$ as this value generated the largest (most negative) DC self-bias and largest electric field reversal for accelerating electrons into the feature. That said, the consequences of voltage waveform tailoring (VWT) on etched features are dominated by the change in the IEADs. Although VWT does produce EEADs with higher energy and narrower angular spread, the effect of these electrons on the feature compared to thermal electrons is not large. This smaller impact of VWT produced EEADs is attributed to thermal electrons being accelerated into the feature by electric fields produced by the positive in-feature charging.

Published under an exclusive license by the AVS. https://doi.org/10.1116/6.0002290

反応モデルのデータベース
QDB

Quantemol database (QDB)

OPEN ACCESS
IOP Publishing
Plasma Sources Science and Technology
Plasma Sources Sci. Technol. 31 (2022) 095020 (28pp)
https://doi.org/10.1088/1361-6595/ac907e

The 2021 release of the Quantemol database (QDB) of plasma chemistries and reactions

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[13] School of Physical Sciences, Faculty of Science and Health, Dublin City University, Dublin, Ireland

Abstract

The Quantemol database (QDB) provides cross sections and rates of processes important for plasma models; heavy particle collisions (chemical reactions) and electron collision processes are considered. The current version of QDB has data on 28 917 processes between 2485 distinct species plus data for surface processes. These data are available via a web interface or can be delivered directly to plasma models using an application program interface; data are available in formats suitable for direct input into a variety of popular plasma modeling codes including HPEM, COMSOL, ChemKIN, CFD-ACE+, and VisGlow. QDB provides ready assembled plasma chemistries plus the ability to build bespoke chemistries. The database also provides a Boltzmann solver for electron dynamics and a zero-dimensional model. These developments, use cases involving O_2, Ar/NF_3, $Ar/NF_3/O_2$, and $He/H_2O/O_2$ chemistries, and plans for the future are presented.

Keywords: atomic and molecular data, chemistries, plasma models, low temperature plasmas

Q-VT(HPEM), COMSOL, CHEMKIN, CFD-ACE+, VizGlow 等の商用コードに import 可能

複数のデータベースに見つかる約 10,000 のデータを機械学習

Rate Coefficient Calculator

The Quantemol team has developed a machine learning regression model to rapidly estimate reaction rate coefficients for heavy particle collisions. The model was trained on approximately 10,000 instances of kinetic data obtained from four popular plasma process databases: QDB [1], NFRI [2], KIDA [3], and UDfA [4]. The model features were engineered from commonly available data that describe individual chemical species involved in the reactions, such as molar masses, charges, enthalpies of formation, dipole moments, polarizabilities, and elemental composition data.

The final prediction algorithm is a voting regressor that combines distinct, optimised machine learning regressors, including support vector regressor [5], random forest regressor [6], gradient-boosted trees regressor [6, 7], and k-nearest neighbours regressor [8].

An evaluation of the prediction algorithm was performed on a dataset containing over 1000 test reactions. It was discovered that, for more than 87% of these reactions, the predicted rate coefficient values had an error of less than one order of magnitude. Please note, the prediction error for certain reactions was significantly higher.

We invite all users to benefit from this model and populate your chemistry sets with missing data for heavy particle reactions.

However, it is important to keep in mind that while machine learning models can offer fast predictions, they may not be as accurate as more complex calculations like quantum chemistry methods. Therefore, the results obtained with machine learning models should be treated with a certain degree of scepticism.

Please enter the chemical reaction that you wish to investigate. Please note:

- Elements are case-sensitive, e.g. Ar,O,CH4,HCl
- Ions are specified by + or -, eventually followed by the charge number, e.g. H+, Cl-, Ar+2
- Species are separeted by ' + ' and reactants and products are separated by ' -> '. Please mind the spaces between the species and these symbols.
- Reaction rate coefficient only works for two reactant-product pairs e.g 'Ar+ + H2O -> Ar + H2O+' or for reactions with three products e.g 'O3 + HO2 -> O2 + O2 + OH'

Reaction: SUBMIT RESET

QDB (cont.)

※ QGM で Reduced model を構築

OPEN ACCESS
IOP Publishing
Plasma Sources Science and Technology
Plasma Sources Sci. Technol. 29 (2021) 125024 (19pp)
https://doi.org/10.1088/1361-6595/abcd53

Fast species ranking for iterative species-oriented skeletal reduction of chemistry sets

Martin Hanicinec[1], Sebastian Mohr[2] and Jonathan Tennyson[1,*]

[1] Department of Physics and Astronomy, University College, London, Gower St., London, WC1E 6BT, United Kingdom
[2] Quantemol Ltd, 320 City Road, London, EC1V 2NZ, United Kingdom

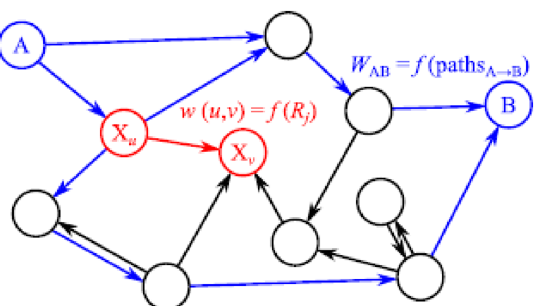


Figure 3. Depiction of a *chemistry graph* with nodes representing species and directional edges representing asymmetric direct interactions between species, weighted by the direct interaction coefficients. A direct interaction coefficient $w(u, v)$ between uth and vth species is depicted in red, while the asymmetric coupling coefficient W_{AB} between species A and B is hinted in blue, depending on all the paths $p(A \to B)$ in the chemistry graph leading from A to B.

Abstract

A fast algorithm is developed for ranking the species in a chemistry set according to their importance to the modeled densities of user-specified species of interest. The species ranking can be constructed for any set of user-specified plasma conditions, but here we focus predominantly on low-temperature plasmas, with gas temperatures between 300 and 1500 K covering the typical range of ICP and CCP plasma sources. This ranking scheme can be used to acquire insight into complex chemistry sets for modeling plasma phenomena or for a species-oriented reduction of the given chemistry set. The species-ranking method presented is based on a graph-theoretical representation of the detailed chemistry set and establishing indirect asymmetric coupling coefficients between pairs of species by the means of widely used graph search algorithms. Several alternative species-ranking schemes are proposed, all building on the theory behind different flavors of the directed relation graph method. The best-performing ranking method is identified statistically, by performing and evaluating a species-oriented iterative skeletal reduction on six, previously available, test chemistry sets (including O_2–He and N_2–H_2) with varying plasma conditions. The species-ranking method presented leads to reductions of between 10 and 75% in the number of species compared to the original detailed chemistry set, depending on the specific test chemistry set and plasma conditions.

Keywords: plasma modeling, chemistry reduction, species ranking, chemistry graph

ATHENASYS

Quantemol Global model (QGM) Ar/O2/C4F6/C4F8 mixture の例

Set Generation | Chemistry Set | Boltzmann Solver | Model Settings | Results | Analysis

85 species are selected. **85 species**

		Name	Sticking Coefficient	Return Coefficient	Ret
☑	Properties	Ar	0.0000	0.0000	Ar
☑	Properties	Ar+	1.0000	1.0000	Ar
☑	Properties	Ar2+	1.0000	2.0000	Ar
☑	Properties	Ar3+	1.0000	3.0000	Ar
☑	Properties	Ar[**]	1.0000	1.0000	Ar
☑	Properties	Ar[*]	1.0000	1.0000	Ar
☑	Properties	Ar[3*]	1.0000	1.0000	Ar
☑	Properties	C	0.0000	0.0000	C

☑ Auto-Add Reactions

Add Custom Species

Add QDB Species

Filtering

Filtering
- ☐ Show only selected species
- ☑ Ground State Neutrals
- ☑ Excited States
- ☑ Positive Ions
- ☑ Negative Ions

Excited States
- ◉ Use pooled states
- ○ Use distinct states

885 reactions are selected. **885 reactions**

		Reaction	A	n	E	Thresh
☑	Info	O + O- > e- + O2	2.30e-10	0.00	0.00	0.00
☑	Info	e- + O2 > O + O-	1.39e-09	-1.37	6.77	0.00
☑	Info	e- + C2F5 > CF3- + CF2	5.34e-09	-1.44	3.8.	0.00
☑	Info	Ar + Ar+ > Ar + Ar+	5.66e-10	0.50	0.00	0.00
☑	Info	e- + Ar2+ > Ar + Ar[*]	2.20e-05	-0.64	0.00	0.00
☑	Info	e- + Ar > e- + Ar	3.67e-07	-0.11	3.49	0.00

Backward Forward

Add Reaction

☑ Auto-Update Species

☐ Show only selected reactions

Filter by Type
- ☑ show electron collisions
- ☑ show heavy particle collisions

Filter by Reactants
- ☐ Has Reactants

Ar, Ar+, Ar2+, Ar3+, Ar[**], Ar[*], Ar[3*], C, C+, C-, C2

Filter by Products
- ☐ Has Products

Ar, Ar+, Ar2+, Ar3+, Ar[**], Ar[*], Ar[3*], C, C+, C-, C2

☑ Enable Consistency Checks **Consistency Checks**

Some Ion-Ion Recombination reactions are missing! Show

Some symmetric charge exchange reactions are missing! Show

The following species are not produced by any gas phase reactions:
C4F6 : Produced only at surfaces

The following species are not consumed by any gas phase reactions:
C2F2 : No loss channels in gas phase or at surfaces C3F4 : No loss channels in gas phase or at surfaces C3F+ : Consumed only at surfaces C3F2+ : Consumed only at surfaces C3F3+ : Consumed only at surfaces
C3F4+ : Consumed only at surfaces C4F4+ : Consumed only at surfaces C4F5+ : Consumed only at surfaces C4F6+ : Consumed only at surfaces COF2+ : Consumed only at surfaces
CF3[v=*] : Consumed only at surfaces

Save Set

QGM (cont.) reduced model（※AMAT の検討例）

$Ar/NF_3/O_2$ and Ar/NF_3 plasmas

Modeling of Inductively Coupled $Ar/NF_3/O_2$ and Ar/NF_3 Plasmas

Shahid Rauf
Applied Materials, Inc., Santa Clara, CA, USA

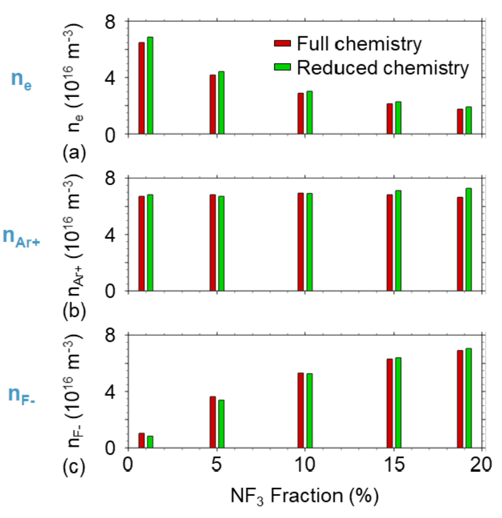
2023 Quantemol Workshop
London, England
April 14, 2023

概要：

主要な species と反応式を抽出し，Species の数を 2/3 程度，反応式を 1/3 程度に低減して，ほぼ同等の結果を得ることに成功

Spatially-Averaged Charged Species Densities

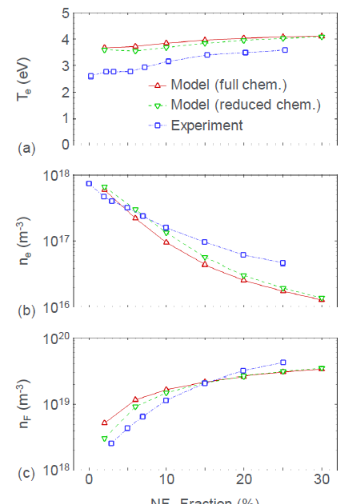
- The full and reduced chemistries capture the trends in charged species vs. NF_3 / O_2 fraction in the gas mixture. Densities are also quantitatively close.
- n_e decreases with increasing NF_3 fraction in the gas mixture due to the high electronegativity of NF_3.
- Density of the dominant negative ion, F^-, increases with increasing NF_3 fraction in the gas mixture.



- 140 W, 30 mTorr, $Ar/NF_3/O_2$ = 80/x/20-x

Model Validation in Ar/NF_3

- The computed n_e and T_e at (*r*, *z*) = (0, 4.5) cm are compared to measurements in Ar/NF_3 plasma.
- In addition, spatially-averaged F density is compared to actinometry-based measured density.
- F recombination coefficient (F → F_2 on surfaces) was adjusted (0.004) based on experimental validation.
- The model captures the experimental trends in these quantities:
  - Ne decreases with increasing NF_3 fraction due to enhanced electronegativity
  - F density increases with NF_3 fraction due to more F availability
- Plasma chemistry mechanism has too many "degrees of freedom" to attempt a better match.



- 140 W, 30 mTorr, Ar/NF_3 = 100-*x*/*x*

電子衝突断面積の推算ツール
QEC

電子衝突断面積の推算ツール：Quantemol-EC (QEC)

QEC Tutorial: an overview（8分弱）
https://www.youtube.com/watch?v=pKYEVNbK5z4

Article

Quantemol Electron Collisions (QEC): An Enhanced Expert System for Performing Electron Molecule Collision Calculations Using the R-Matrix Method

Bridgette Cooper [1], Maria Tudorovskaya [2], Sebastian Mohr [2], Aran O'Hare [1], Martin Hanicinec [1], Anna Dzarasova [2], Jimena D. Gorfinkiel [3], Jakub Benda [3], Zdeněk Mašín [4], Ahmed F. Al-Refaie [1], Peter J. Knowles [5] and Jonathan Tennyson [1,*]

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Abstract: Collisions of low energy electrons with molecules are important for understanding many aspects of the environment and technologies. Understanding the processes that occur in these types of collisions can give insights into plasma etching processes, edge effects in fusion plasmas, radiation damage to biological tissues and more. A radical update of the previous expert system for computing observables relevant to these processes, Quantemol-N, is presented. The new Quantemol Electron Collision (QEC) expert system simplifyies the user experience, improving reliability and implements new features. The QEC graphical user interface (GUI) interfaces the Molpro quantum chemistry package for molecular target setups, and the sophisticated UKRmol+ codes to generate accurate and reliable cross-sections. These include elastic cross-sections, super elastic cross-sections between excited states, electron impact dissociation, scattering reaction rates, dissociative electron attachment, differential cross-sections, momentum transfer cross-sections, ionization cross sections, and high energy electron scattering cross-sections. With this new interface we will be implementing dissociative recombination estimations, vibrational excitations for neutrals and ions, and effective core potentials in the near future.

Keywords: cross sections; elastic scattering; inelastic scattering; electronic excitation; rotational excitation; electron scattering; ionization; momentum transfer

QEC (続き)

Underlying Codes：UK-RMOL+

What does Quantemol-EC do?

Calculates a variety of observables for electron molecule collisions including:
Zero – high electron energy extension for all cross sections*

- Elastic cross-sections
- Electronic excitation cross-sections
- Super-elastic/Quenching cross-sections
- Electron impact dissociation
- Scattering reaction rate
- Arrhenius parameters for reaction rates
- Resonance parameters
- Estimate dissociative electron attachment*
- Differential cross-sections
- Momentum transfer cross-sections
- Electron impact ionisation at all energies*
- Cross-sections for oriented molecules
- Rotational excitation cross-sections
- Vibrational excitation (non resonant)*
- Effective Core potentials for ionisation
- Approximation of electron scattering from condensed state: turning off long range moments in the outer region of the calculation

* features not present in standard R-matrix codes

Computer Physics Communications
Volume 249, April 2020, 107092

CPC 50th anniversary article

UKRmol+: A suite for modelling electronic processes in molecules interacting with electrons, positrons and photons using the R-matrix method ☆

Zdeněk Mašín [a], Jakub Benda [b], Jimena D. Gorfinkiel [b], Alex G. Harvey [c], Jonathan Tennyson [d]

Show more

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https://doi.org/10.1016/j.cpc.2019.107092   Get rights and content

What range of problems can be tackled with Quantemol-EC?

- Closed shell molecules
- Open shell molecules, radicals
- Neutral and positively charged species
- Large molecules (up to 25 atoms, preferably lighter than Ar)

QEC (続き)

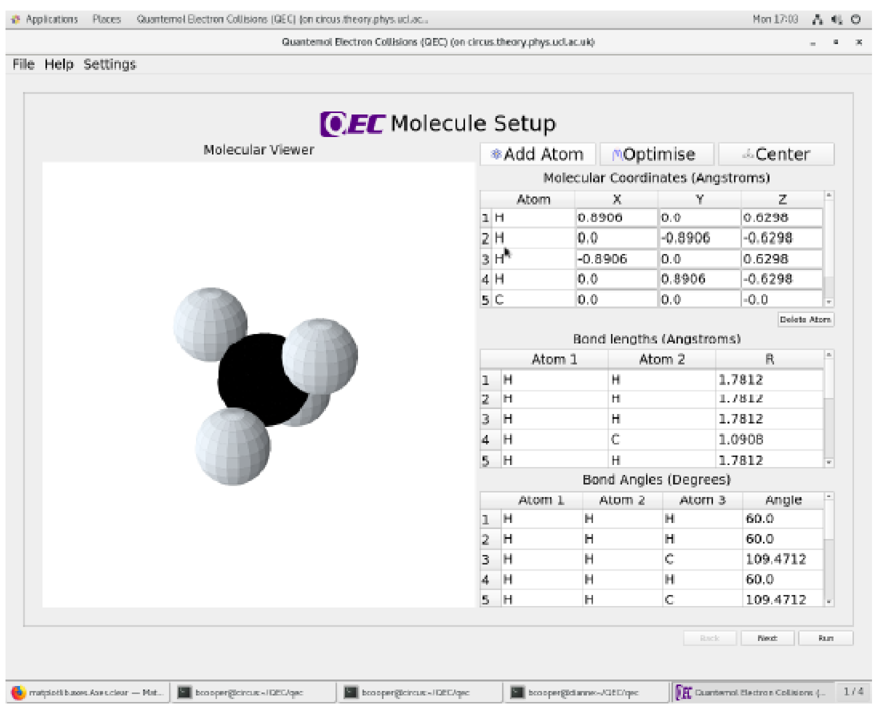

Figure 1. Screenshot of the molecular set-up page in the Quantemol Electron Collision (QEC) graphical user interface (GUI) showing methane as an example. The screenshot was taken after the geometry had been optimized using Molpro and the coordinates automatically shifted to the center of mass.

※ Molpro とセットで利用
※ Ubuntu 等，Linux 環境が必要

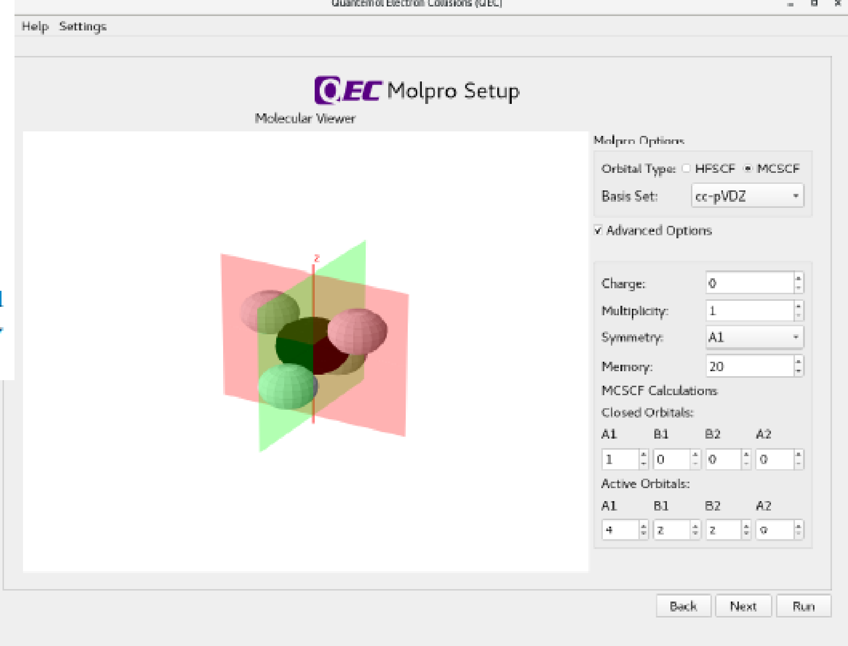

Figure 2. Screenshot of the page in the QEC GUI which sets up the molecular target calculation which is performed using Molpro.

QEC (続き)： ※ 計算結果の一例

Graphical Display

BEB ionisation cross-section

Cross Section (Å²)

Energy (eV)

x - Axis: linear / logarithmic

y - Axis: linear / logarithmic

Close Save

File Help Settings

Calculation Log

```
Finished the inner region.

Starting the matrix outer
Number of final symmetries i
Finished final symmetry 1 of
Time taken = 0.74 s.
Expected remaining time = 2
Finished final symmetry 2 of
Time taken = 1.17 s.
Expected remaining time = 0
Finished final symmetry 3 of
Time taken = 1.61 s.
Expected remaining time = 0
Finished final symmetry 4 of
Time taken = 1.89 s.

Finished the outer region
Arrhenius parameters for el
/scratch/bcooper/Sept_onwa
Skipping dissociative attac
Skipping high energy elasti

Calculating differential, mo
Time taken for Polydcs (s)
Finished running Polydcs
Arrhenius parameters for Mo
/scratch/bcooper/Sept_onwa
Arrhenius parameters for In
/scratch/bcooper/Sept_onwar
Skipping calculation of exc
Skipping vibrational excita

Calculation completed succe
2021-01-04 14:21:00
Time taken for this calcula
```

Graphical Display

Rotational Excitation Cross-section

Cross-section ($\times 10^{-16}$cm²)

Energy (eV)

0 --> 1
0 --> 2
0 --> 3
0 --> 4
0 --> 5

x axis: linear / logarithmic

y axis: linear / logarithmic

Close Save

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興味がありましたら，以下にお問合せ下さい。

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