Uncertainty quantification of theoretical atomic and molecular collisional data

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Fusion requires a huge set of AM data

Mostly Theoretical Data Available

EFDA TASK Force

INTEGRATED TOKAMAK MODELLING

AM processes for kinetic modelling of H

1) e-induced atomic elastic $e + H \rightarrow e + H$ [16]R. Celloberto, et al., Atomic Data2) e-induced atomic ionization $e + H \rightarrow 2e + H^+$ [16]3) e-induced vibrational excitation eV $e + H_2(\nu) \rightarrow e + H_2(w)$ [16]4) e-induced vibrational excitation EV $e + H_2(\nu) \rightarrow e + H_2(w) + h\nu$ [16]5) molecular ionization $e + H_2(\nu) \rightarrow e + H_2^+$ [16]6) dissociative ionization $e + H_2(\nu) \rightarrow e + H_2^+$ [16]7) dissociative ionization $e + H_2(\nu) \rightarrow e + H_2^+$ [16]8) molecular electronic excitation $e + H_2(\nu) \rightarrow e + H_2^+$ [16]9) dissociative attachment $e + H_2^+ \rightarrow 2H + H^+$ [16]10) molecular assisted recombination MAR $e + H_2^+ \rightarrow 2H + H^+$ [17]11) mlecular assisted of dissociation MAD $e + H_2^+ \rightarrow 2e + 2H^+$ [17]12) molecular assisted ionization MAI $e + H_2^+ \rightarrow 2e + 2H^+$ [17]13) p-induced atomic elastic $H^+ + H_2(\nu) \rightarrow H^+ + H_2(w)$ [18]14) p-induced dissociation $H^+ + H_2(\nu) \rightarrow H^+ + H_2(w)$ [19]15) ion conversion $H^+ + H_2(\nu) \rightarrow H^+ + H_2(\nu)$ [17]14) p-induced dissociation $H^+ + H_2(\nu) \rightarrow H^+ + H_2(\nu)$ [17]15) collision induced dissociation $H^+ + H_2(\nu) \rightarrow H^+ + H_2(\nu)$ [17]16) celtron detachment $H^- + H^ 2H$ [17]17) charge exchange with molecule $H^- + H^ 2H$ [17]19) collision induced dissociation $H^- + H^ 2H$ [17]10) electron detachment with atom $H^- + H^ 2H$ [17]11) charge exchange wit	Volume Processees	Reaction Formulas	Ref.	[16] D. Calibarta et al. Atamia Data
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13) p-induced atomic elastic $H^+ + H \leftrightarrow H^+ + H$ [18]14) p-induced elastic/vibrational excitation $H^+ + H_2(\nu) \leftrightarrow H^+ + H_2(w)$ [18]15) ion conversion $H^+ + H_2(\nu) \rightarrow H_2^+ + H$ [18]16) p-induced dissociation $H^+ + H_2(\nu) \rightarrow H^+ + 2H$ [18]17) charge exchange with atom $H_2^+ + H \rightarrow H^+ + H_2(\nu)$ [19]18) charge exchange with molecule $H_2^+ + H_2(\nu) \rightarrow H_2(w) + H_2^+$ [17]19) collision induced dissociation $H_2^+ + H_2(\nu) \rightarrow H^+ + H_2(\nu)$ [17]20) electron detachment $H^- + H^- \rightarrow 2H$ [17]21) charge exchange recombination $H^- + H \rightarrow H_2(\nu) + e$ [17]22) electron detachment with atom $H^- + H \rightarrow H_2(\nu) + e$ [17]23) electron detachment with molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]23) electron detachment with molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]23) electron detachment with molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]24) electron detachment with molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]25) electron detachment with molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]26) electron detachment with molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]27) electron detachment with molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]21) charge exchange recombination $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]21) charge exchange two molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]21) charge exchange two molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]22) electron	12) molecular assisted ionization MAI	$e + H_2^+ \rightarrow 2e + 2H^+$	[17]	Atomic Data Center, ORNL,
14) p-induced elastic/vibrational excitation $H^+ + H_2(\nu) \leftrightarrow H^+ + H_2(w)$ [18]15) ion conversion $H^+ + H_2(\nu) \rightarrow H_2^+ + H$ [18]16) p-induced dissociation $H^+ + H_2(\nu) \rightarrow H^+ + 2H$ [18]17) charge exchange with atom $H_2^+ + H \rightarrow H^+ + H_2(\nu)$ [19]18) charge exchange with molecule $H_2^+ + H_2(\nu) \rightarrow H_2(w) + H_2^+$ [17]19) collision induced dissociation $H_2^+ + H_2(\nu) \rightarrow H^+ + H + H_2(\nu)$ [17]20) electron detachment $H^- + H^- \rightarrow 2e + H$ [17]21) charge exchange recombination $H^- + H^+ \rightarrow 2H$ [17]22) electron detachment with atom $H^- + H \rightarrow H_2(\nu) + e$ [17]23) electron detachment with molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]23) electron detachment with molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]10) electron detachment with molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]11) charge exchange recombination $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]12) electron detachment with atom $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]13) electron detachment with molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]147 - 152 (2008) / DOI10 1002/eterp 200810026	13) p-induced atomic elastic	$\mathrm{H^{+}} + \mathrm{H} \leftrightarrow \mathrm{H^{+}} + \mathrm{H}$	[18]	Tennessee, 1990).
15) ion conversion $H^+ + H_2(\nu) \rightarrow H_2^+ + H$ [18]16) p-induced dissociation $H^+ + H_2(\nu) \rightarrow H^+ + 2H$ [18]17) charge exchange with atom $H_2^+ + H \rightarrow H^+ + H_2(\nu)$ [19]18) charge exchange with molecule $H_2^+ + H_2(\nu) \rightarrow H_2(w) + H_2^+$ [17]19) collision induced dissociation $H_2^+ + H_2(\nu) \rightarrow H^+ + H + H_2(\nu)$ [17]20) electron detachment $H^- + e \rightarrow 2e + H$ [17]21) charge exchange recombination $H^- + H^+ \rightarrow 2H$ [17]22) electron detachment with atom $H^- + H \rightarrow H_2(\nu) + e$ [17]23) electron detachment with molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]147 - 152 (2008) / DOI10 1002/eterp 200810026	14) p-induced elastic/vibrational excitation	$\mathrm{H^{+}} + \mathrm{H}_{2}(\nu) \leftrightarrow \mathrm{H^{+}} + \mathrm{H}_{2}(w)$	[18]	
16) p-induced dissociation $H^+ + H_2(\nu) \rightarrow H^+ + 2H$ [18]17) charge exchange with atom $H_2^+ + H \rightarrow H^+ + H_2(\nu)$ [19]18) charge exchange with molecule $H_2^+ + H_2(\nu) \rightarrow H_2(w) + H_2^+$ [17]19) collision induced dissociation $H_2^+ + H_2(\nu) \rightarrow H^+ + H + H_2(\nu)$ [17]20) electron detachment $H^- + e \rightarrow 2e + H$ [17]21) charge exchange recombination $H^- + H^+ \rightarrow 2H$ [17]22) electron detachment with atom $H^- + H \rightarrow H_2(\nu) + e$ [17]23) electron detachment with molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]147 - 152 (2008) / DOI10 1002/otem 200810026	15) ion conversion	$\mathrm{H^+} + \mathrm{H_2}(\nu) \rightarrow \mathrm{H_2^+} + \mathrm{H}$	[18]	"Plasma-Neutral Interaction in
17) charge exchange with atom $H_2^+ + H \rightarrow H^+ + H_2(\nu)$ [19]18) charge exchange with molecule $H_2^+ + H_2(\nu) \rightarrow H_2(w) + H_2^+$ [17]19) collision induced dissociation $H_2^+ + H_2(\nu) \rightarrow H^+ + H + H_2(\nu)$ [17]20) electron detachment $H^- + e \rightarrow 2e + H$ [17]21) charge exchange recombination $H^- + H^+ \rightarrow 2H$ [17]22) electron detachment with atom $H^- + H^+ \rightarrow 2H$ [17]23) electron detachment with molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]147 - 152 (2008) / DOI10 1002/eterp 200810026	16) p-induced dissociation	$\mathrm{H^+} + \mathrm{H_2}(\nu) \rightarrow \mathrm{H^+} + 2\mathrm{H}$	[18]	Kinetic Models for the Divertor
18) charge exchange with molecule $H_2^+ + H_2(\nu) \rightarrow H_2(w) + H_2^+$ [17]19) collision induced dissociation $H_2^+ + H_2(\nu) \rightarrow H^+ + H + H_2(\nu)$ [17]20) electron detachment $H^- + e \rightarrow 2e + H$ [17]21) charge exchange recombination $H^- + H^+ \rightarrow 2H$ [17]22) electron detachment with atom $H^- + H \rightarrow H_2(\nu) + e$ [17]23) electron detachment with molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]10) electron detachment with molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]11) charge exchange recombination $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]12) electron detachment with molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]147 - 152 (2008) / DOI10 1002 (atops 200810026)	17) charge exchange with atom	$H_2^+ + H \rightarrow H^+ + H_2(\nu)$	[19]	Region"
19) collision induced dissociation $H_2^+ + H_2(\nu) \rightarrow H^+ + H + H_2(\nu)$ [17]20) electron detachment $H^- + e \rightarrow 2e + H$ [17]21) charge exchange recombination $H^- + H^+ \rightarrow 2H$ [17]22) electron detachment with atom $H^- + H \rightarrow H_2(\nu) + e$ [17]23) electron detachment with molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]10) electron detachment with molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]11) the detachment with molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]12) electron detachment with molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]147 - 152 (2008) / DOI10 1002 (atops 200810026)	18) charge exchange with molecule	$H_2^+ + H_2(\nu) \to H_2(w) + H_2^+$	[17]	E Taccogna B Schneider K
20) electron detachment $H^- + e \rightarrow 2e + H$ [17]21) charge exchange recombination $H^- + H^+ \rightarrow 2H$ [17]22) electron detachment with atom $H^- + H \rightarrow H_2(\nu) + e$ [17]23) electron detachment with molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]10) $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]11) $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17]12) electron detachment with molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ 12) electron detachment with molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ 12) electron detachment with molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ 12) electron detachment with molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ 13) electron detachment with molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ 14) H_2(\nu) = H^- + H_2(\nu) + e[17]14) H_2(\nu) = H^- + H_2(\nu) + e[18]14) H_2(\nu) = H^- + H_2(\nu) + e[18]14) H_2(\nu) =	19) collision induced dissociation	$\mathrm{H}_{2}^{+} + \mathrm{H}_{2}(\nu) \rightarrow \mathrm{H}^{+} + \mathrm{H} + \mathrm{H}_{2}(\nu)$	[17]	Matvash S Longo M Capitelli
21) charge exchange recombination 22) electron detachment with molecule $ \begin{array}{c} H^- + H^+ \rightarrow 2H \\ H^- + H \rightarrow H_2(\nu) + e \\ H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e \end{array} $ [17] [17] [17] [17] [17] [17] [17] [17]	20) electron detachment	$H^- + e \rightarrow 2e + H$	[17]	and D. Tskhakava
22) electron detachment with atom 23) electron detachment with molecule $ \begin{array}{c} H^- + H \rightarrow H_2(\nu) + e \\ H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e \end{array} $ [17] [17] [17] [147 - 152 (2008) / DOI [10 1002/otep 200810026]	21) charge exchange recombination	$H^- + H^+ \rightarrow 2H$	[17]	Contrib Plasma Phys 48 No. 1-3
23) electron detachment with molecule $H^- + H_2(\nu) \rightarrow H + H_2(\nu) + e$ [17] 147 – 152 (2008) 7 DOT 10 1002/otep 200810026	22) electron detachment with atom	$\mathrm{H^-} + \mathrm{H} \rightarrow \mathrm{H}_2(\nu) + \mathrm{e}$	[17]	147 152 (2008) / DOI
	23) electron detachment with molecule	$\mathrm{H^-} + \mathrm{H_2}(\nu) \rightarrow \mathrm{H} + \mathrm{H_2}(\nu) + \mathrm{e}$	[17]	147 - 152(2000) / DOI

32

Critical Assessment for Modeling of Physical Processes (VVUQ)



- Verification. The process of determining how accurately a computer program ("code") correctly solves equations of the mathematical model.
 - Validation. The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model
- Uncertainty quantification (UQ). The process of quantifying uncertainties associated with model calculations of true, physical QOIs
- For Optimization-based designs of complex systems and components (e.g. divertor), a comprehensive modeling is required and its VVUQ are critical.
- Majority of available data sets required as input parameters for a modeling are theoretical or computational, most of which are not provided with uncertainty.
- UQ, data evaluation and internationally agreed recommended data library for fusion relevant AM/PSI data are long-term objectives of the Unit.

Uncertainties associated with AM data

- UQ less developed for AM data compared to nuclear data AM data look for the solution of an appropriate many-body quantum system with known (Coulombic) interaction compared to nuclear data field reliant on models calibrated to experimental data
- Uncertainty in fundamental parameters outside the domain of atomic and molecular physics

Fine structure constant, electron-to-proton mass ratio, and in nuclear properties, the mass, magnetic dipole moment, electrostatic quadrupole moment and finer details of the charge distribution of nuclei involved in the system under consideration

• Uncertainty in the fundamental equations, before the introduction of a tractable model

Various approximations at the level of the basic equations (relativistic contributions, Born-Oppenheimer approximation etc)

Uncertainties associated with AM data(2)

- Uncertainty in the model for many-body quantum mechanics Non-relativistc many-body Schrödinger equation is intractractable at a fundamental level (Reduced descriptions: HF, DFC, CCC, etc)
- Uncertainty due to discretization of the model equations A finite basis of atomic orbitals for atomic and molecular systems or a Fourier-space discretization in the case of electronic structure calculations for condensed phase (Truncation error)
- Uncertainties beyond the quantum mechanical treatments
 Reduction to classical calculations; for example trajectory calculations
 using Newton's equations for motion of nuclei (molecular dynamics) with
 use of an interaction potential

The representation of the potential is now an important source of uncertainty that is difficult to quantify.

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A starting point



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Topical Review

Uncertainty estimates for theoretical atomic and molecular data

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Abstract



Sources of uncertainty are reviewed for calculated atomic and molecular data that are important for plasma modeling: atomic and molecular structures and cross sections for electron-atom, electron-molecule, and heavy particle collisions. We concentrate on model uncertainties due to approximations to the fundamental many-body quantum mechanical equations and we aim to provide guidelines to estimate uncertainties as a routine part of computations of data for structure and scattering.

Table of Contents

- 1. Introduction
- 2. General Considerations
- 3. Uncertainty estimates for structure computations
 - A. Atoms
 - B. Molecular electronic ground state properties
 - C. Molecular electronic excited state properties
- 4. Uncertainty estimates for electron scattering calculations
 - A.Electron atom / ion scattering
 - B.Electron molecule scattering
- 5. Uncertainty assessment for charge transfer collisions
- 6. Illustrations
 - A.Structure
 - B.Electron atom/ion collisions
 - C.Electron molecule collisions
 - D.Charge transfer collisions
- 7. Summary, Conclusions and Outlook

Atomic and Molecular Structure

- Hydrogen exactly solved for nonrelativistic wave function and energy; uncertainties due to relativistic, QED corrections, finite nuclear size etc
- Non-hydrogen; Electronical Hamiltonian, particle basis sets, electron correlation treatment, Born-Oppenheimer approximation(Molecule)

Focal Point Analysis (FPA)



Electron correlation treatment

- Use a family of basis sets (aug-ccpVXZ etc) which are systematically changed to the completeness,
- 2. Apply lower levels of theory (typically, HF etc) with very extensive basis sets,
- 3. Execute high order correlation treatments
- 4. Examine the added correlation increments.

Ab initio contributions to the first Dissociation energy of $H_2^{16}O$.

		Value	UQ	
Α	CBS CCSD(T) frozen core	43 956	6	
B	Core correlation CCSD(T)	+81	2	
С	All-electron CBS CCSD(T)[=A+B]	44 037	6	
D	Higher order electron correlation	-52	3	
E	CBS FCI [=C+D]	43 985	7	
F	Scalar relativistic correction	-53	3	
G	QED (Lamb shift) correction	+3	1	
Н	Spin-orbit effect	-69.4	1	
I I	Angular momenta coupling, OH	+31.5	0	
J	Sum spin effects, OH [=H+I]	-37.9	1	
K	DBOC, H ₂ O	+35.3	0.5	
L	ZPE H ₂ O	4638.1	0	
Μ	ZPE OH	1850.7	0.5	
Ν	Net ZPE, H ₂ O [=L+M]	2787.4	0.5	
U	Nonadiabatic contribution	0	1	
V	Total MD, H ₂ O [=I+K+N+U]	-2721	1	
	$D_o(H_2O)$ Calc. [=E+V]	41 145	8	
	$(Obs-Calc) DO(H_2O)$	+1	-	

Uncertainties are given in the last column

All values are in cm⁻¹

H.-K. CHUNG et al,

J. Phys. D: Appl. Phys. 49, 363002 (2016).

Collisional AM data

- Uncertainty estimates for scattering data are even less developed than structure data as they should include uncertainties of structures as well as reaction probabilities.
- Scattering dynamics change as a function of collision energy and hence one should apply different methods to calculate data of different energy ranges
- UQ: Choice of Hamiltonian (relativity, QED etc), electron correlation, basis sets and the treatment of exchange effects between the projectile electron and target electrons
- For Molecules: need to consider nuclear motion as well as electron motion (vibrational, rotation, dissociation processes)

UQ of AM Collisional Data

Angle-integrated cross-sections for electron impact excitation of the $3p^{5}4s$ in argon from the ground state($3p^{6}$) ${}^{1}S_{0}$

Convergence with basis sets

Cross sections for *n*-shell selective charge transfer in C⁶⁺ -H(1s) collisions as functions of impact energy <u>Discrepancies due to different</u> <u>approximations</u>

