“a procedure to explore uncertainty and reliability in theoretical cross section data for electron and positron scattering”

Bobby Antony

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Outline

- Need for cross section data
- Theoretical methodology & Sample Results
  - Electron Scattering
  - Positron Scattering
- Uncertainty estimation
  - Benchmarking Data
  - Consistency check
  - Convergence check
  - Sensitivity to input parameters
  - Further plan
- IAMDB

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Theory: Electron scattering*

- **Low Energy Formalism based on R-matrix**
  - Computes differential, momentum transfer and total cross section in the energy range 0.1eV to 10-15 eV
  - The dissociative electron attachment process is qualitatively investigated

- **Spherical Complex Optical Potential (SCOP) Method**
  - Computes elastic ,inelastic and total cross sections for energies above IP up to 105 keV

- **Complex Scattering Potential-ionization contribution (CSP-ic) Method**
  - Computes ionization cross section from inelastic cross section calculated through SCOP method

*Kaur et al., *J Phys B: At. Mol. Opt. Phys.* **49** (2016) 0225202.

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Theory: Positron scattering*

- **Modified SCOP & CSP-ic Methods**
  - Computes ionization cross section from inelastic cross section calculated through SCOP method.

- **Difference between electron and positron interaction:**
  - Positrons are distinguishable from electrons, hence no exchange.
  - The static interaction is repulsive, and
  - The polarization interaction is attractive in nature.
  - **Positronium Formation and Positron annihilation**

* *Singh et al., J. Phys. Chem. A* **120** (2016) 5685.

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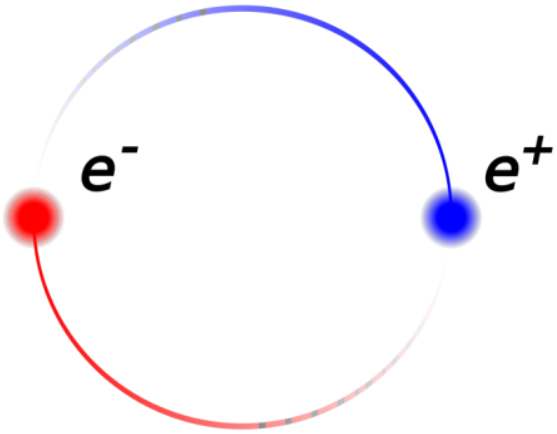
  - The polarization interaction is attractive in nature.

  - **Positronium Formation**
    - **Positronium formation involves the capture of an incident positron by one of the target electrons, to form a "bound state".**
    - **Positronium formation threshold is 6.8 eV below from ionization threshold of the target.**



* Singh et al., *J. Phys. Chem. A* **120** (2016) 5685.

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Results: Electron scattering

- **Electron Scattering Cross Sections**
  - **Differential elastic**
  - **Total elastic**
  - **Momentum transfer**
  - **Electronic excitation**
  - **Total ionization**
  - **Total**

Results: Elastic DCS

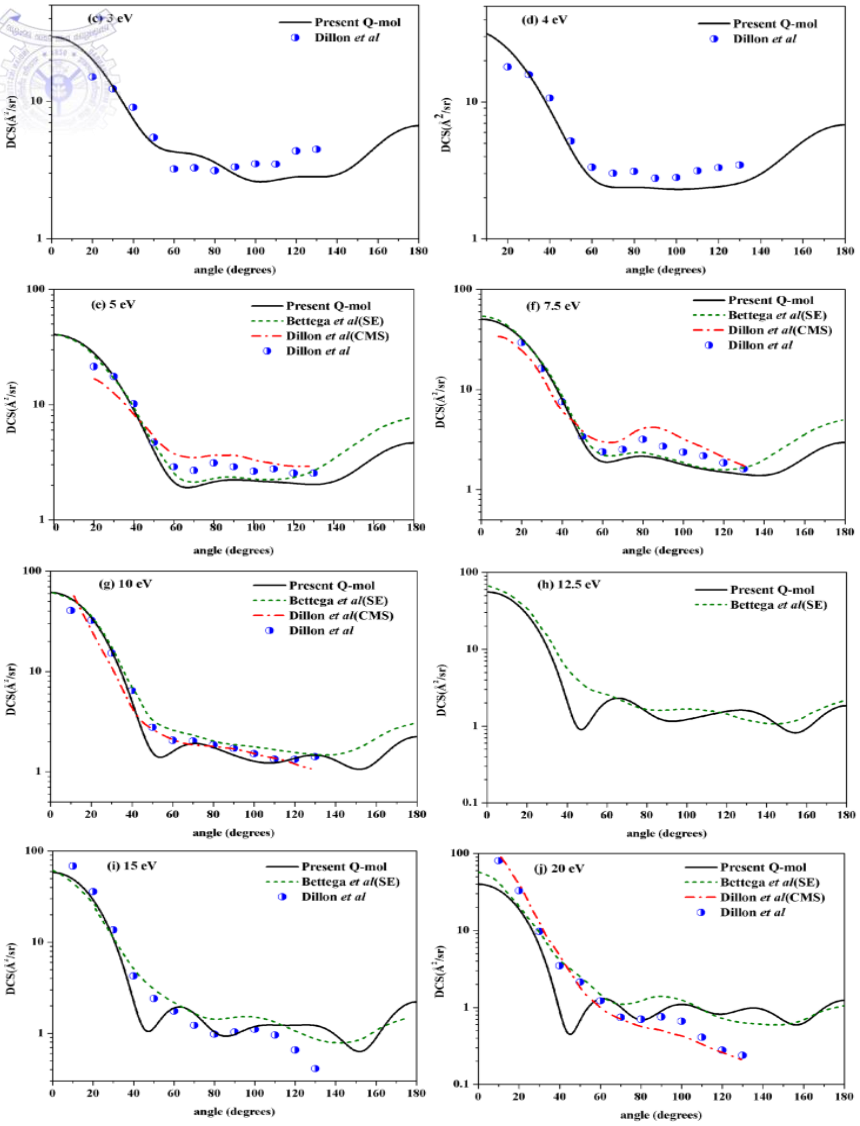


Fig 1: DCS for e-Si_2H_6*

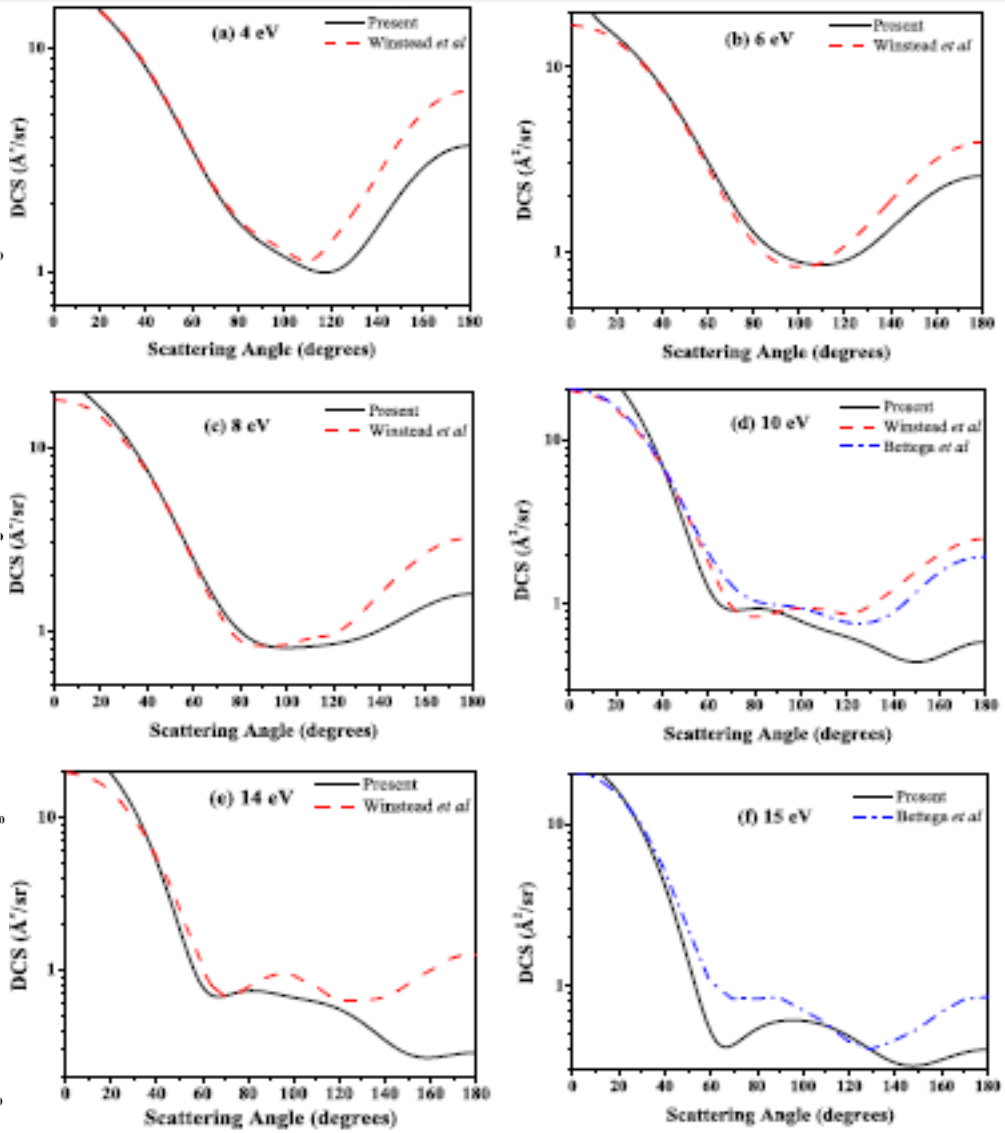


Fig 2: DCS of e-AsH_3#

* Gupta et al. *RSC Adv.* **4** (2014) 9197; # Kaur et al. *Phys. Rev. A* **90** (2014) 012711

Results: Elastic TCS

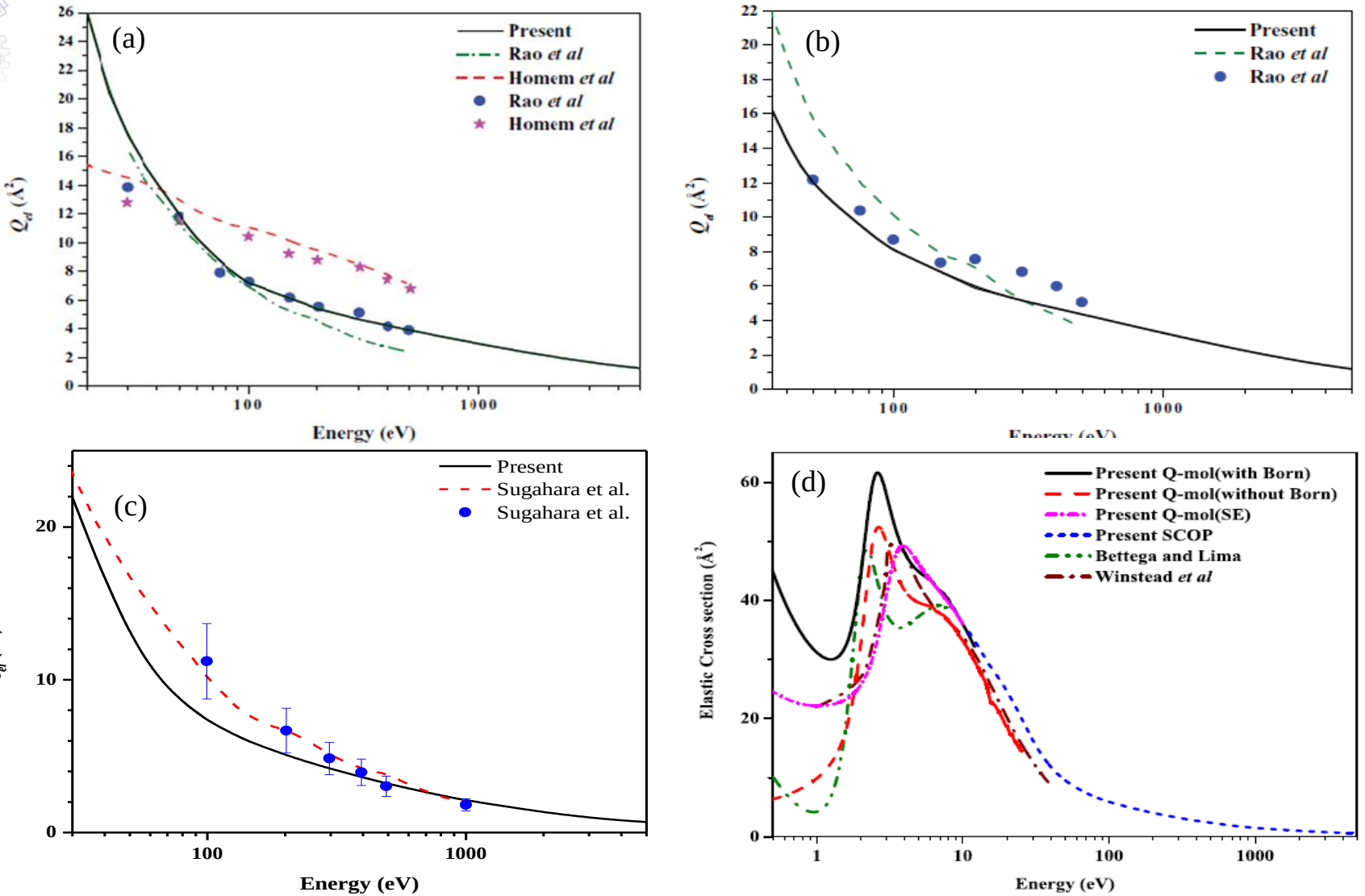


Fig 3: Q_{el} of (a)e-$(CH_3)_2S$*, (b)e-$(CH_3)_2SO$*, (c)e-$(CH_3)_2O$# (d) e-AsH_3 +

* Kaur et al. *Mol. Phys.* **113** (2015) 3883, # Modak et al. *Int. J. Mass Spectrom.* 409 (2016) 1, +Kaur et al. *Phys. Rev. A* **90** (2014) 012711

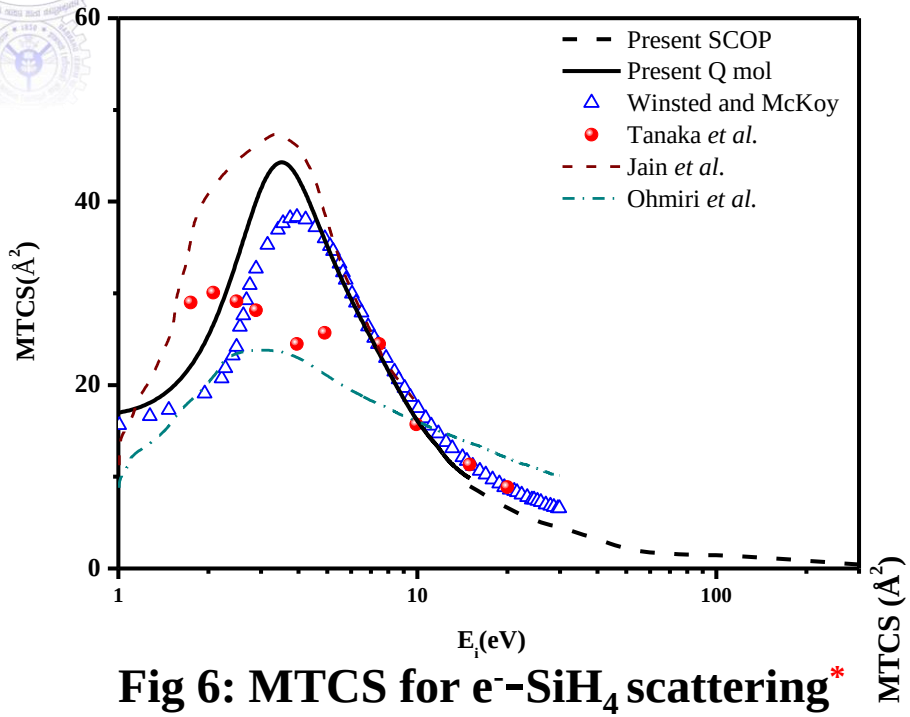


Fig 6: MTCS for e^-–SiH_4 scattering*

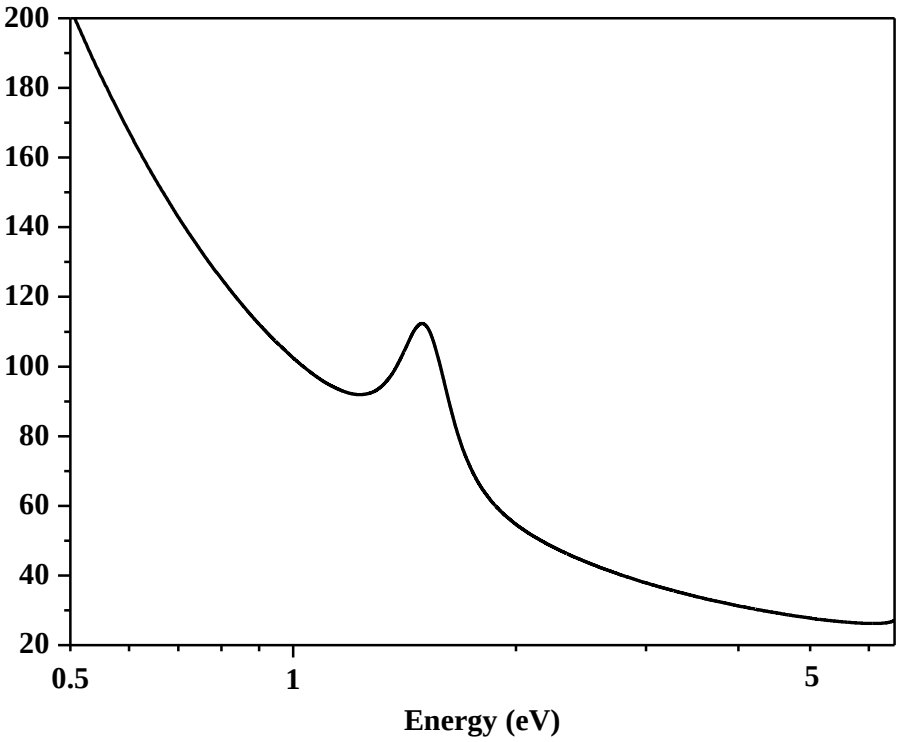


Fig 7: MTCS for e-HCCCN scattering#

* *Verma et al. (2016)*, # *Kaur et al. J Phys B: At. Mol. Opt. Phys. (2016)*

Results: Electronic excitation

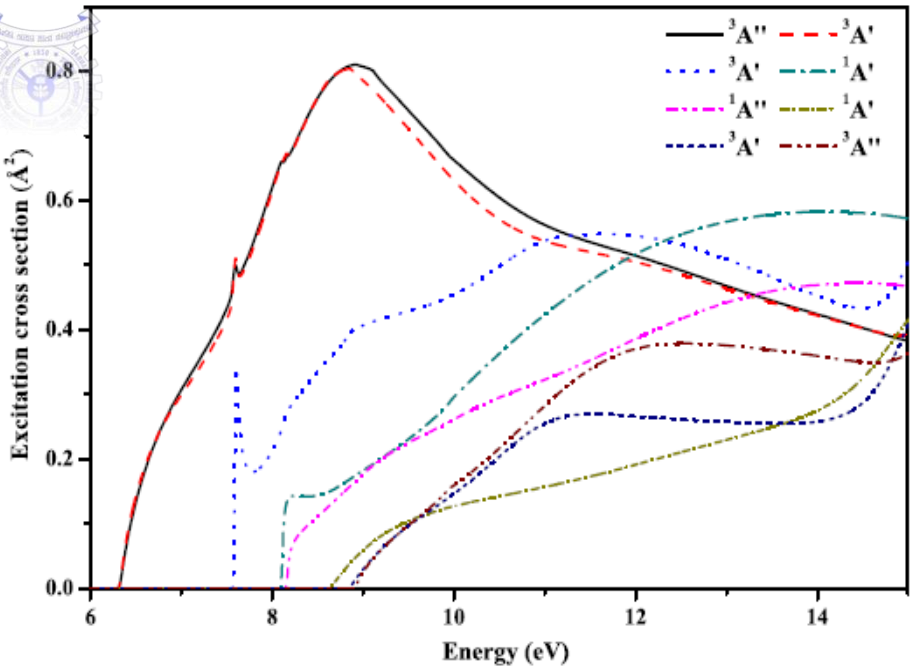


Fig 8: ECS for e-AsH_3 scattering*

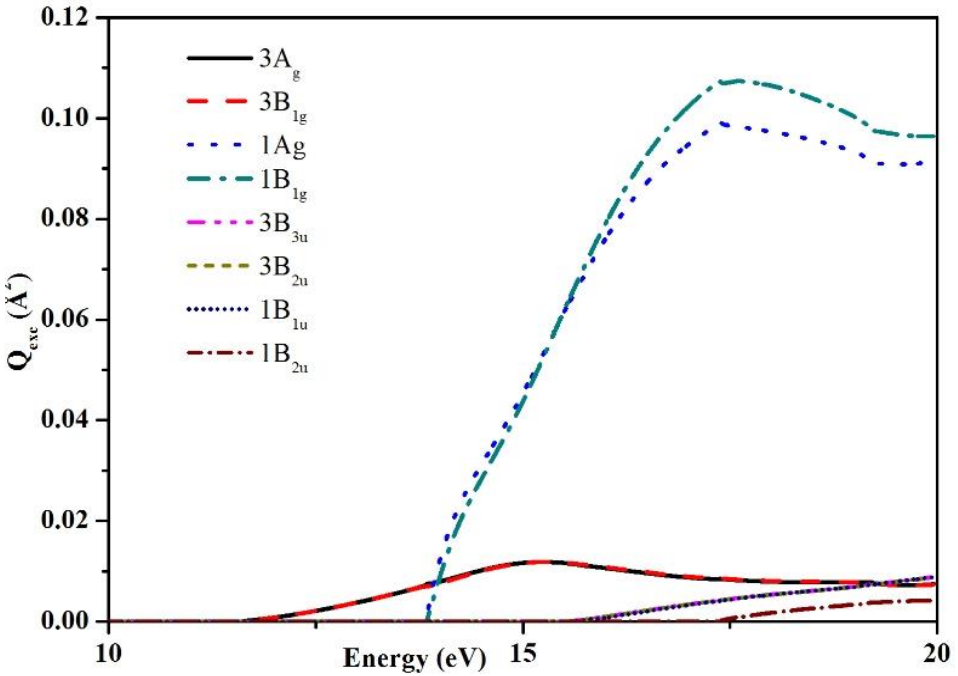


Fig 9: ECS for e-SF_6 scattering#

* Kaur et al. *Phys. Rev. A* **90** (2014) 012711, # Goswami et al. *RSC Adv.* **4** (2014) 30953

Results: Total ionization CS

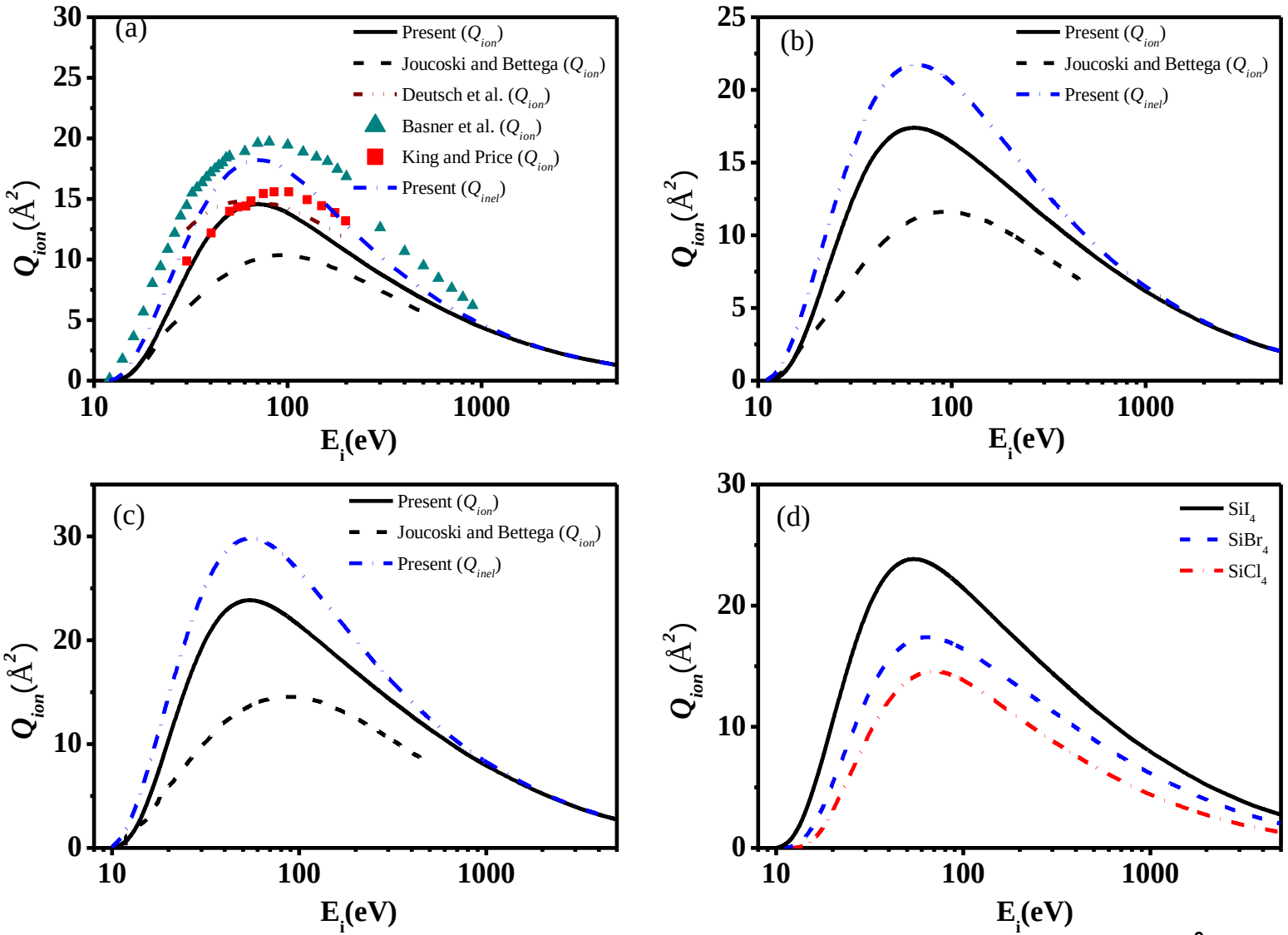


Fig 10: Q_{inel} and Q_{ion} of (a) e-$SiCl_4$, (b) $SiBr_4$, (c) SiI_4 scattering in Å².

* *Verma et al. Phys. Plasmas* **23** *(2016) 093512*

Results: Total ionization CS

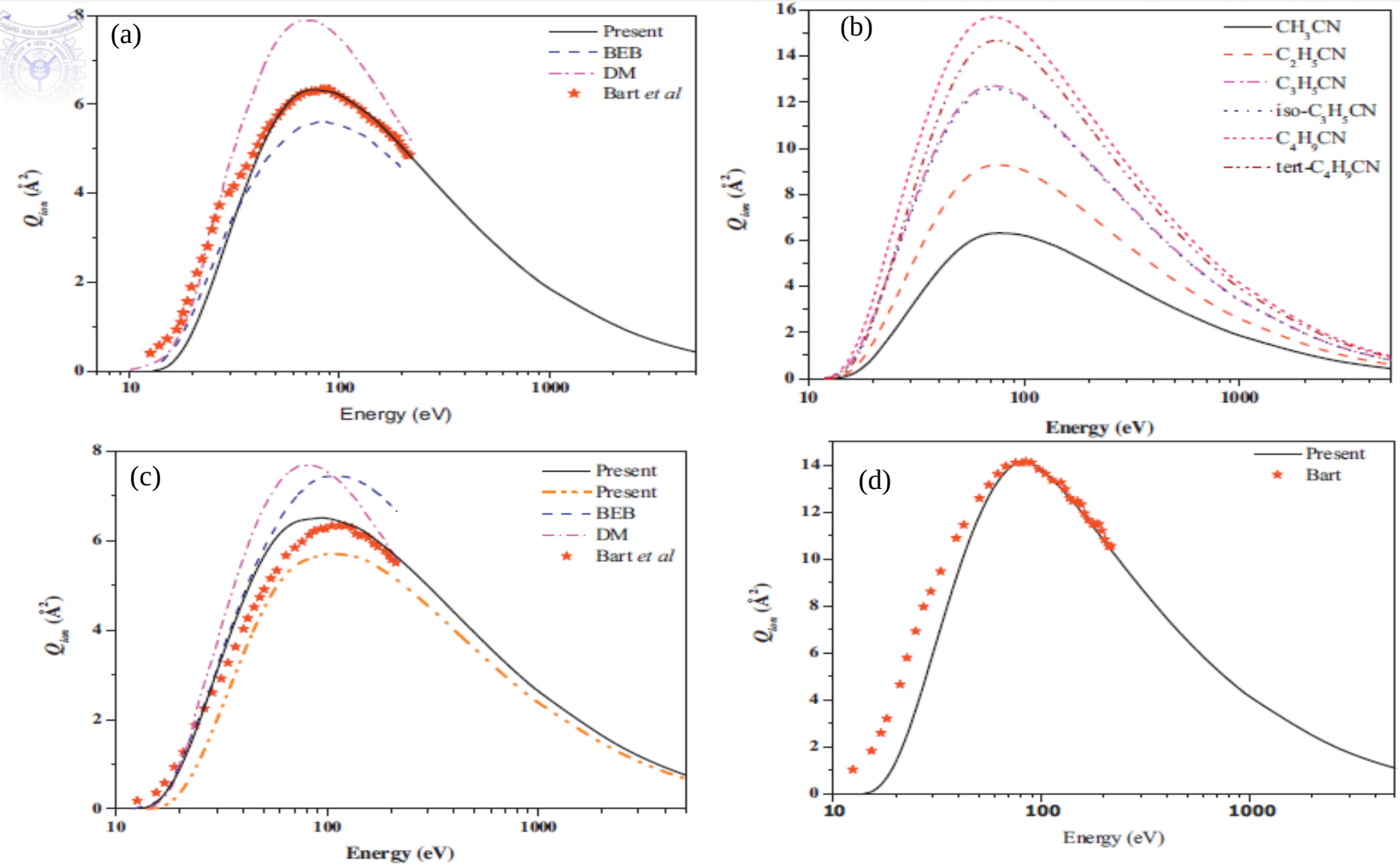


Fig 11*: Q_{ion} of (a) e-CH_3CN, (b) e-$C_nH_{2n-1}CN$; n=1-4, (c) e-CF_3CN (d) e-CCl_3CN

* *Kaur et al. Int. J. Mass. Spectrom,* ***386*** *(2015) 24.*

Results: Total ionization CS

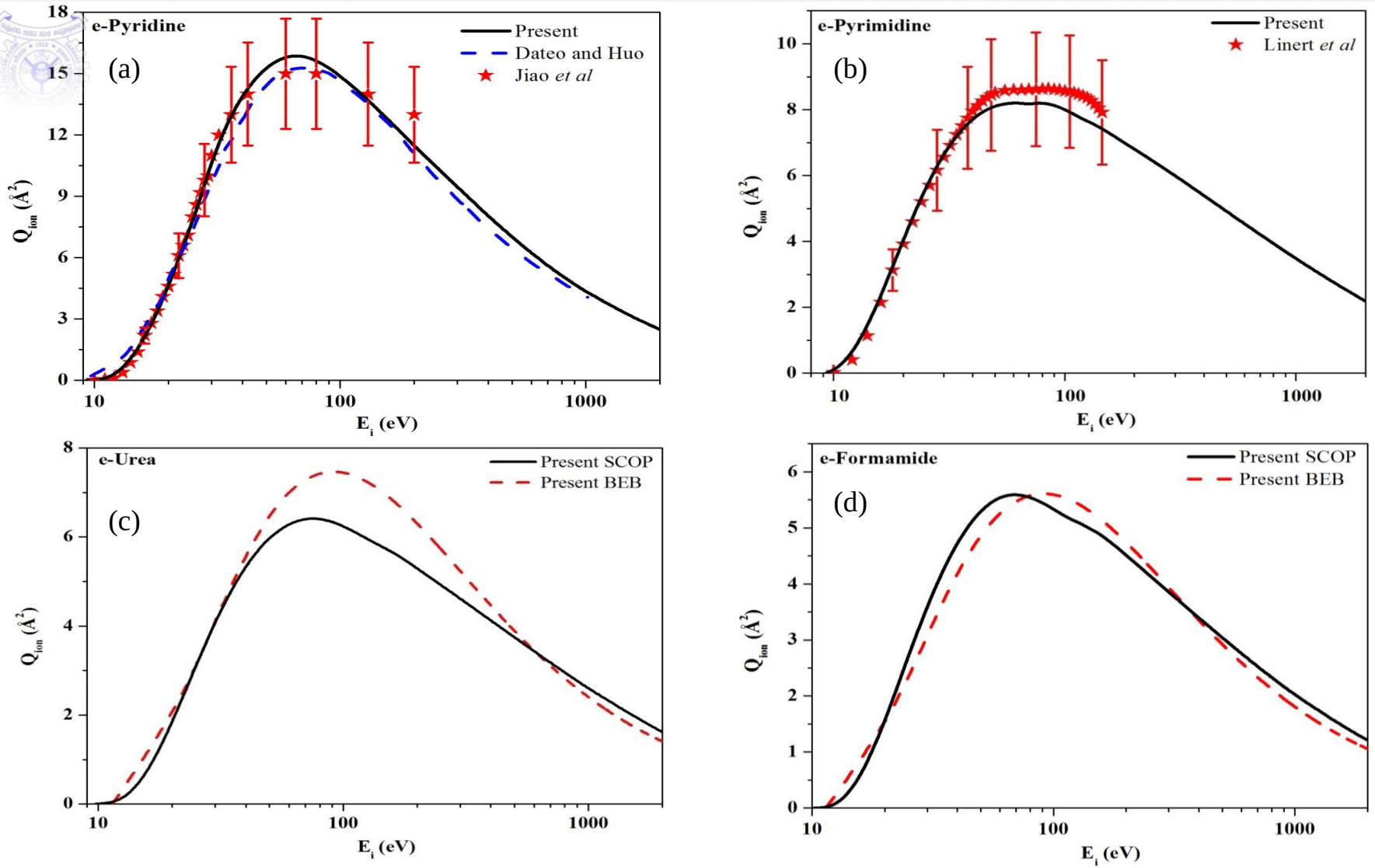
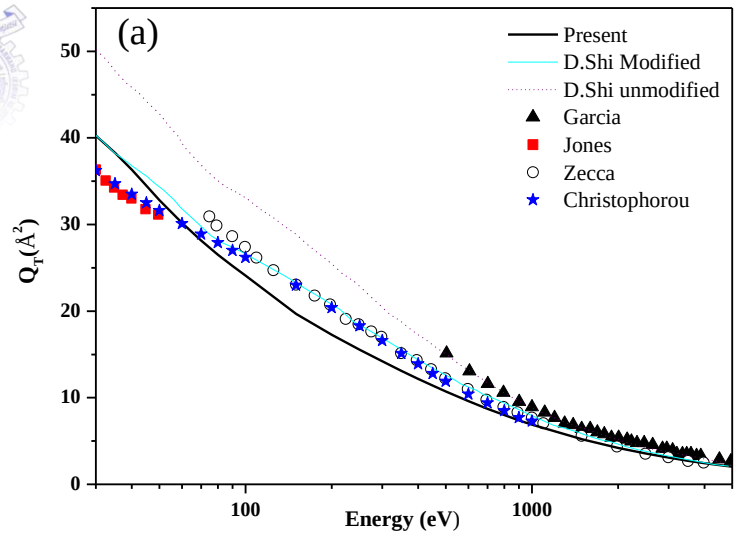
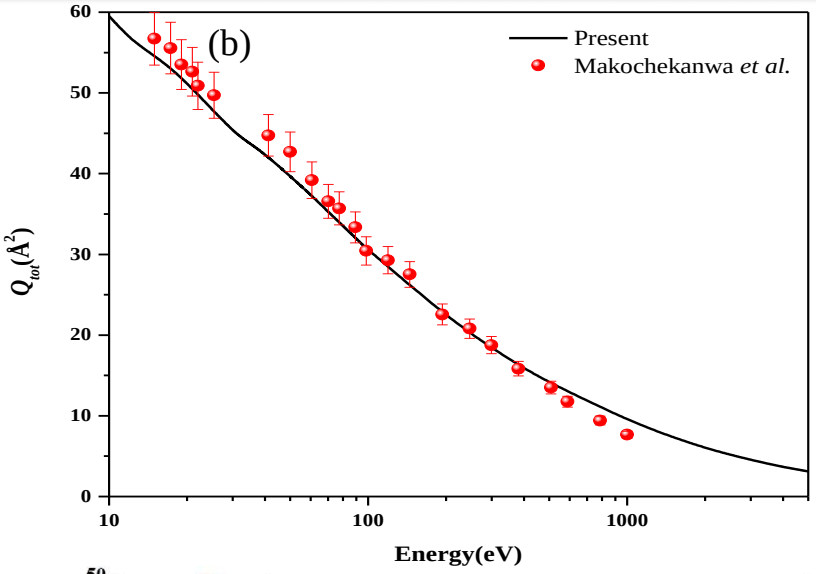


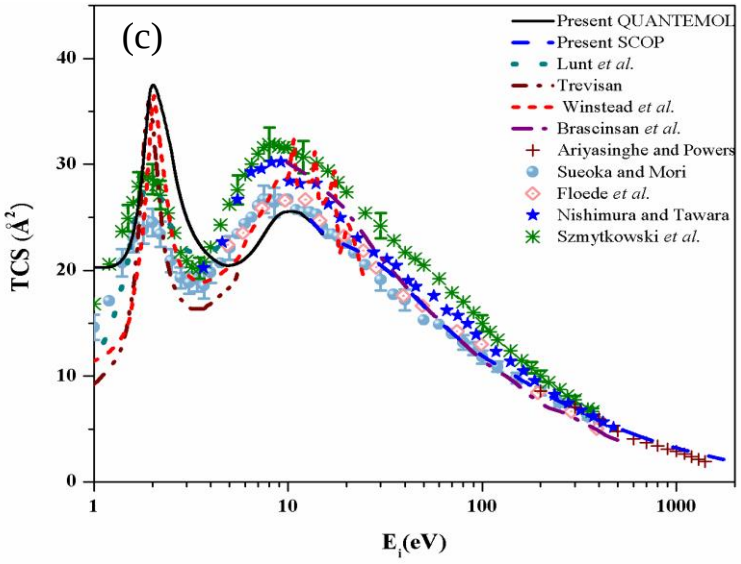
Fig. 12: Q_{ion} of (a) e-Pyridine, (b) e-Pyrimidine, (c) e-Urea (d) e-Formamide scattering*

* *Gupta et al. Mol. Phys.* ***128*** *(2014) 1201.*

Results: Total CS







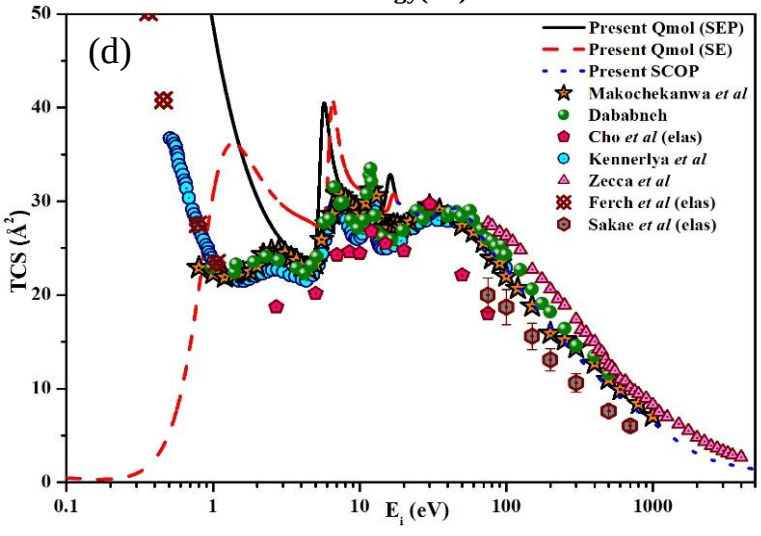


Fig. 13: Q_T of (a) *e-CF_2Cl_2, (b) #e-$(C_nH_{2n-1})_2S$; n=1-3, (c) e-C_2H_4* (d) @ e-SF_6

*Verma et al. J. Elec. Spec. Rel. Phen. **210** (2016) 30 #Kaur et al. Mol. Phys. **113** (2015) 3883 @Singh et al. J. Chem. Phys. **145**(2016) 034309.

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Results: Positron scattering

- **Positron Scattering Cross Sections**
  - **Direct ionization**
  - **Positronium formation**
  - **Total ionization**
  - **Total cross section**

Results: Direct ionization CS

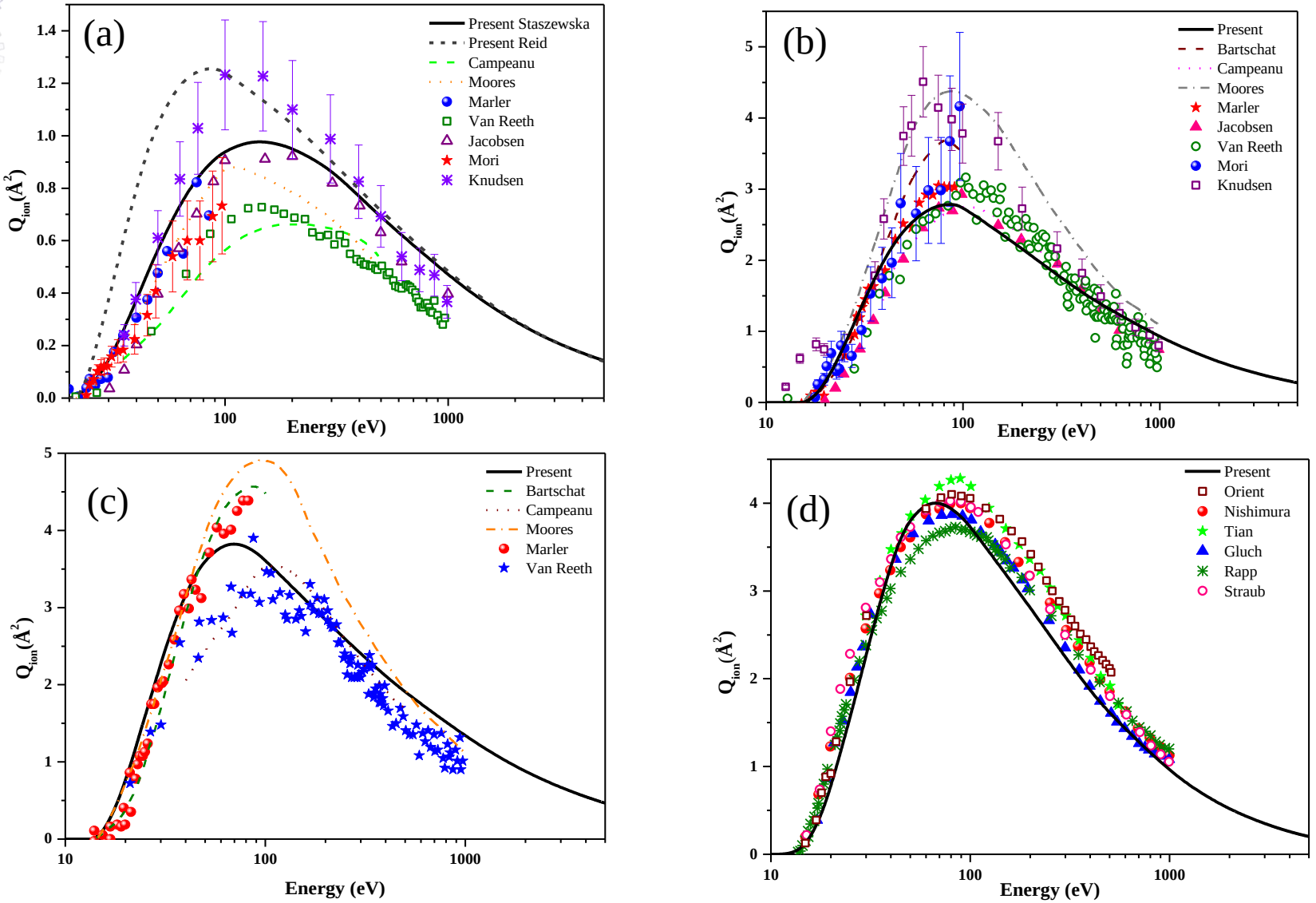
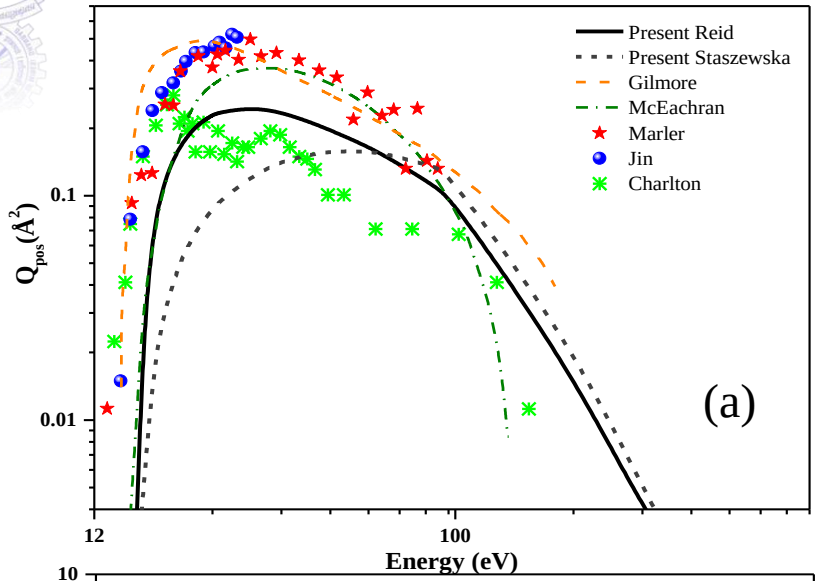
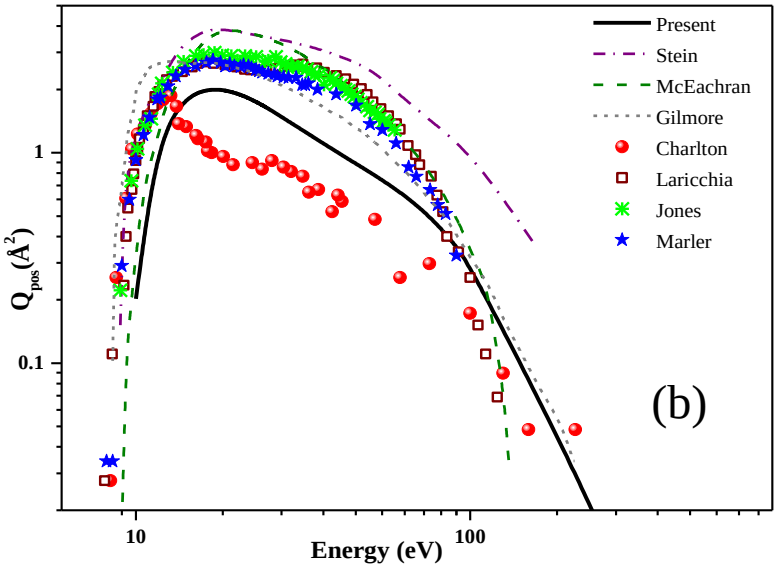


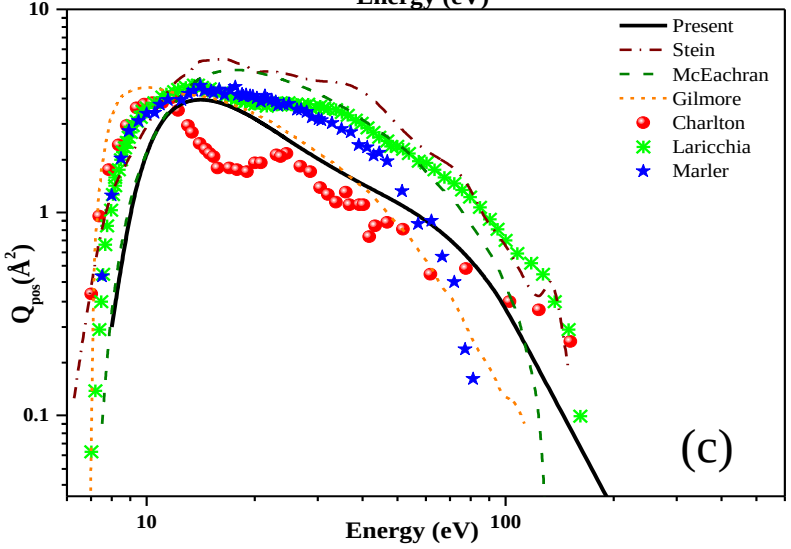
Fig 16: Q_{ion} of (a) e^+-Ne, (b) e^+-Ar, (c) e^+-Kr (d) e^+-CH_4

Unpublished data

Results: Positronium formation CS







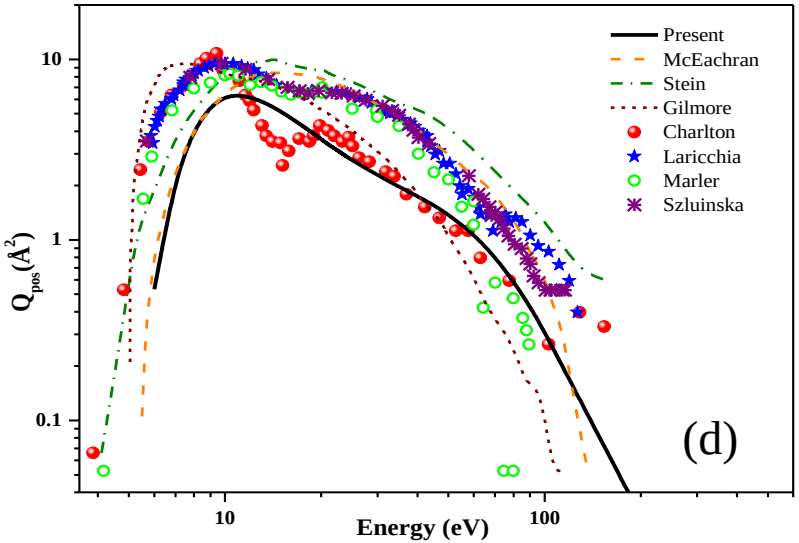


Fig 17: Q_{pos} of (a) e^+-Ne, (b) e^+-Ar, (c) e^+-Kr (d) e^+-Xe scattering .

Unpublished data

Results: Total ionization CS

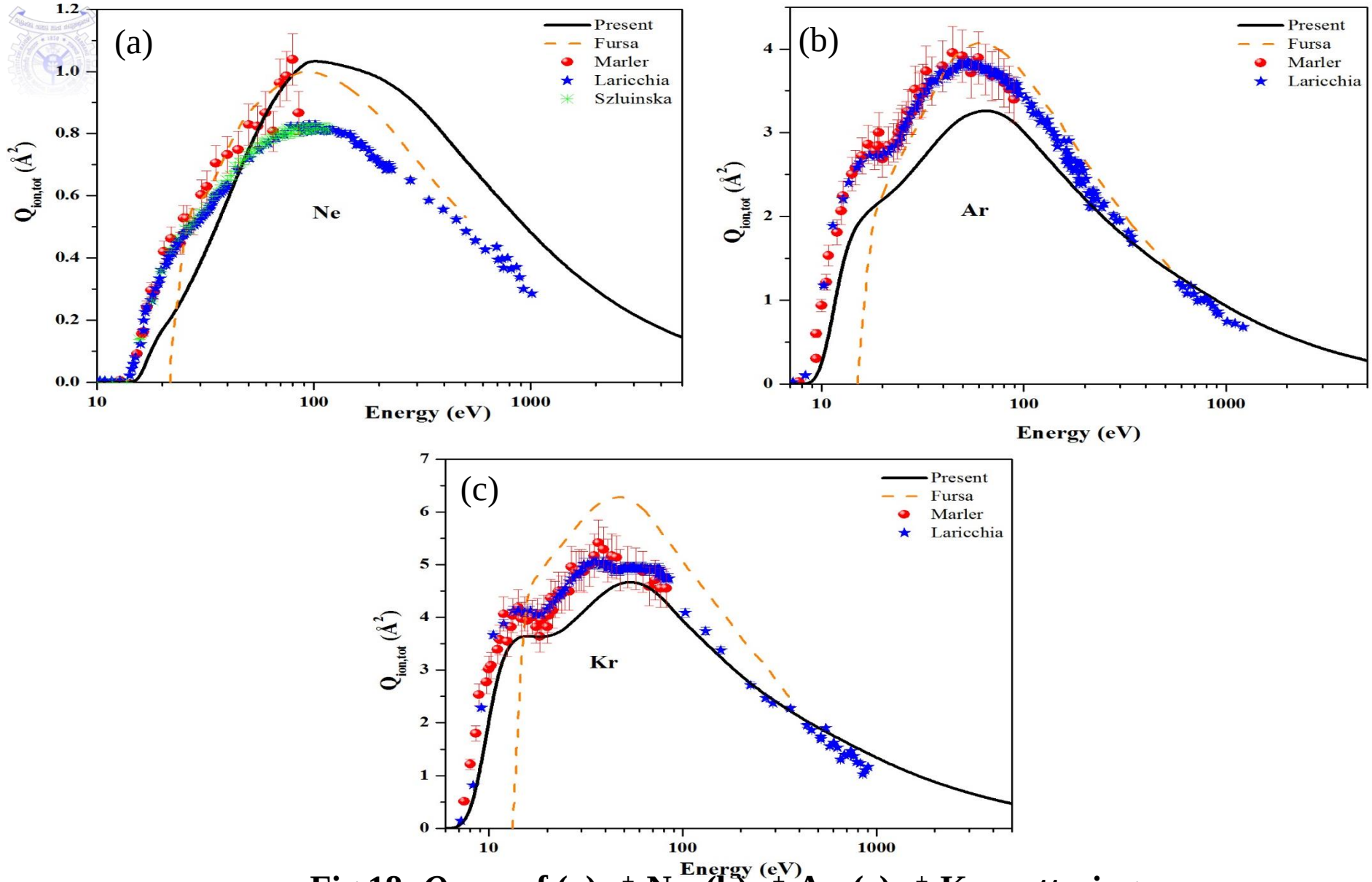


Fig 18: $Q_{ion,tot}$ of (a) e^+-Ne, (b) e^+-Ar, (c) e^+-Kr scattering

Unpublished data

Results: Total CS

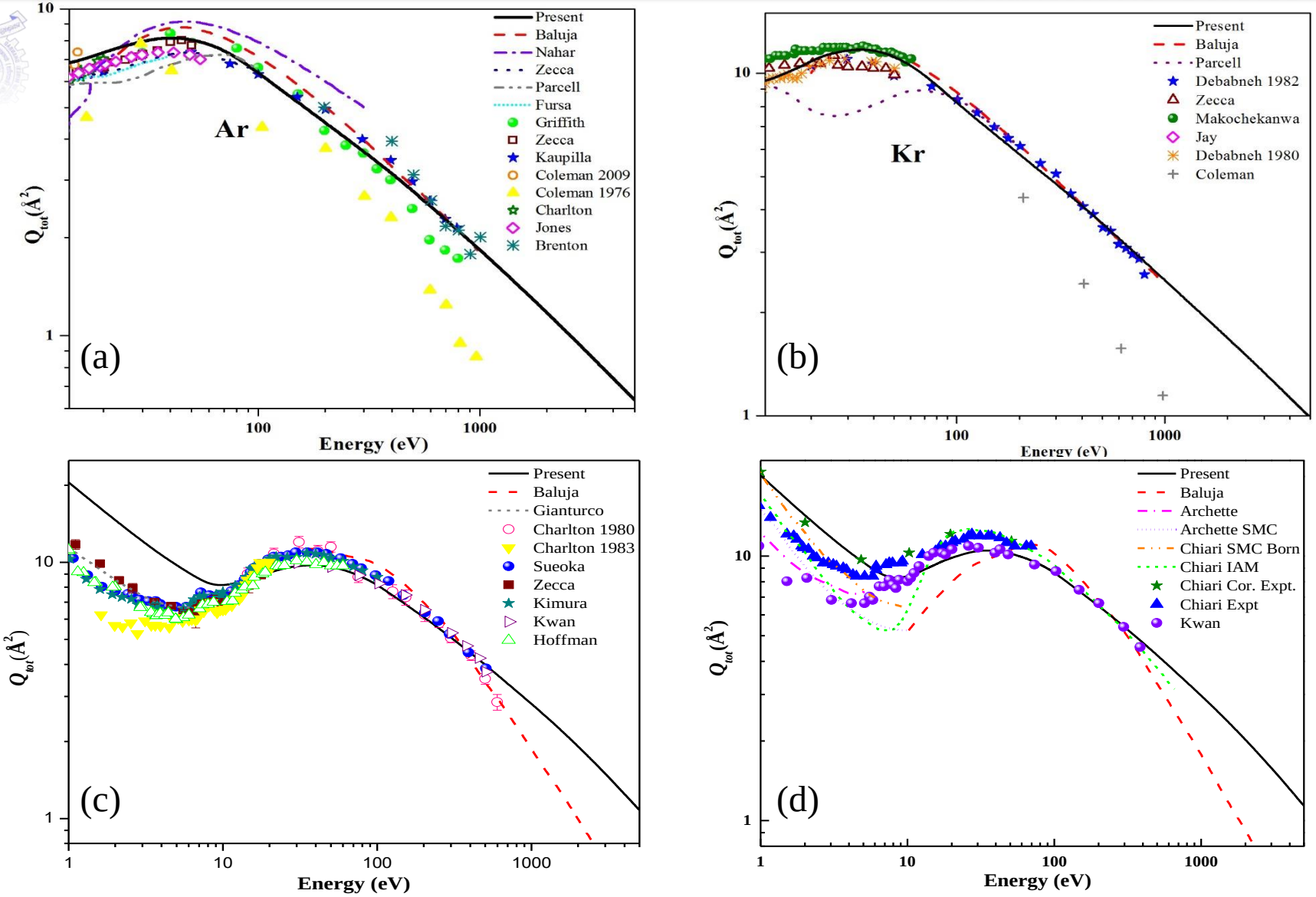


Fig 19: Q_{tot} for (a) e^+-Ar (b) e^+-Kr (c) $^*e^+$-CO and (d) $^*e^+$-NO scattering in Å^2

* *Singh et al., J. Phys. Chem. A* **120** *(2016) 5685.*

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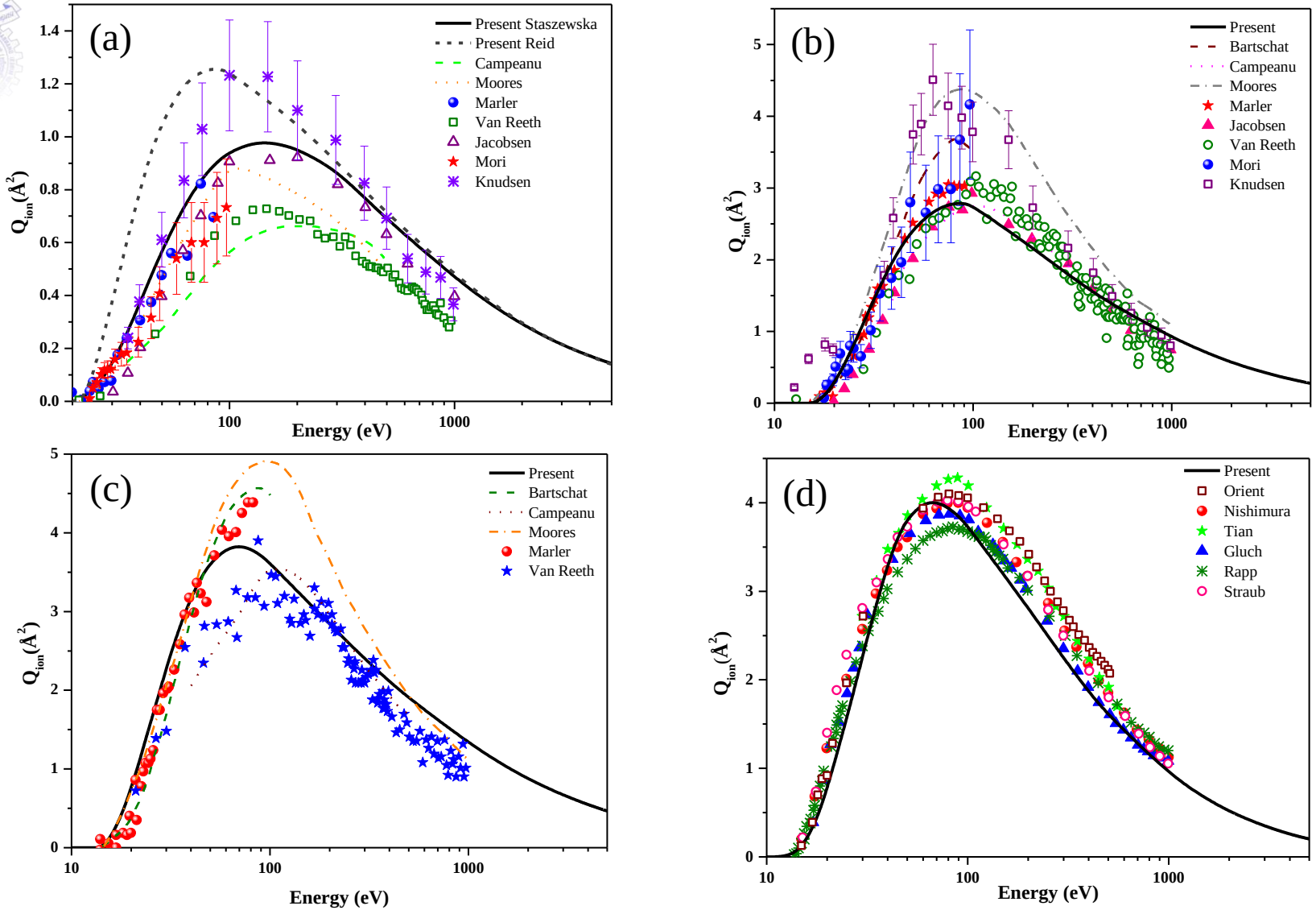
Uncertainty: Benchmarking data



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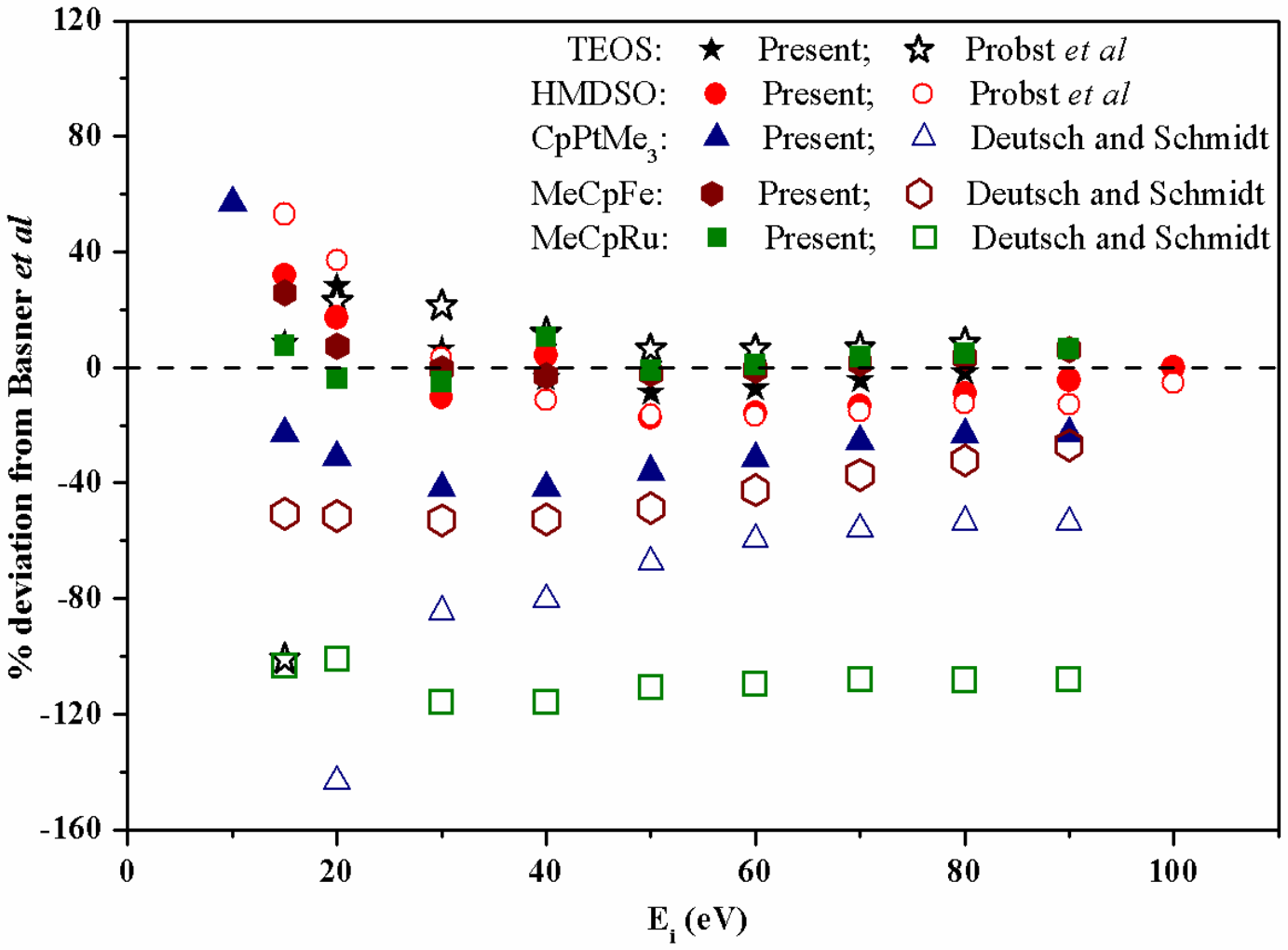
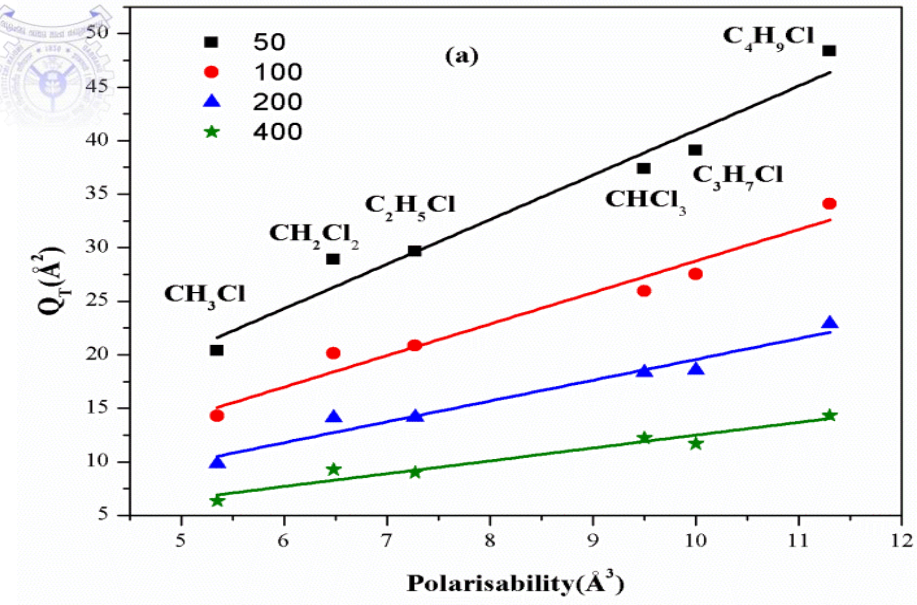
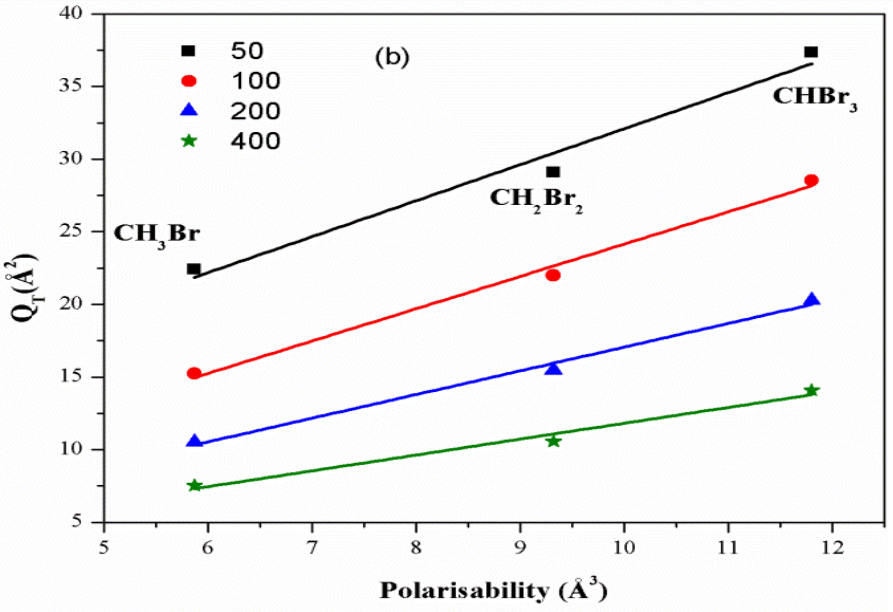
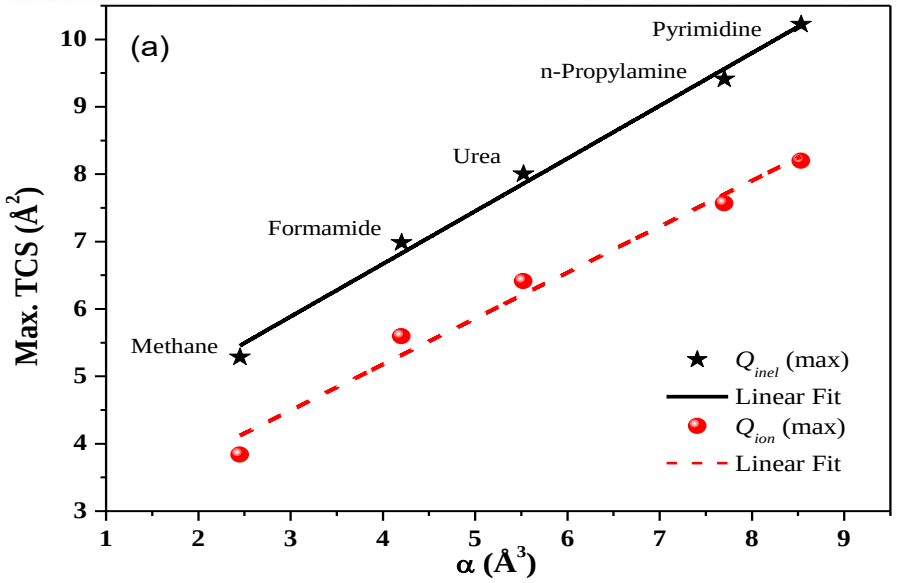


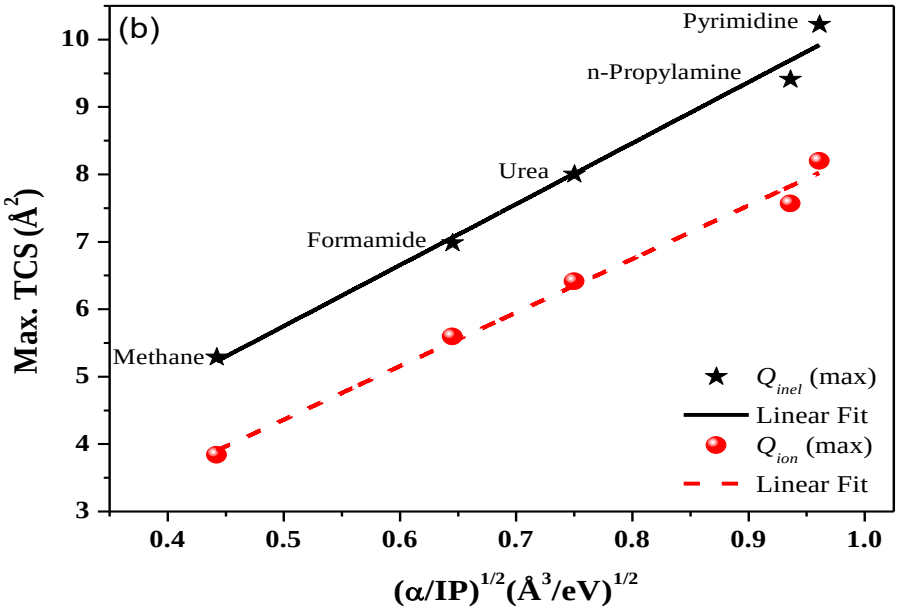
Fig. 17: Deviation of theoretical results from the experiments (organometallic compounds)

Uncertainty: Consistency check

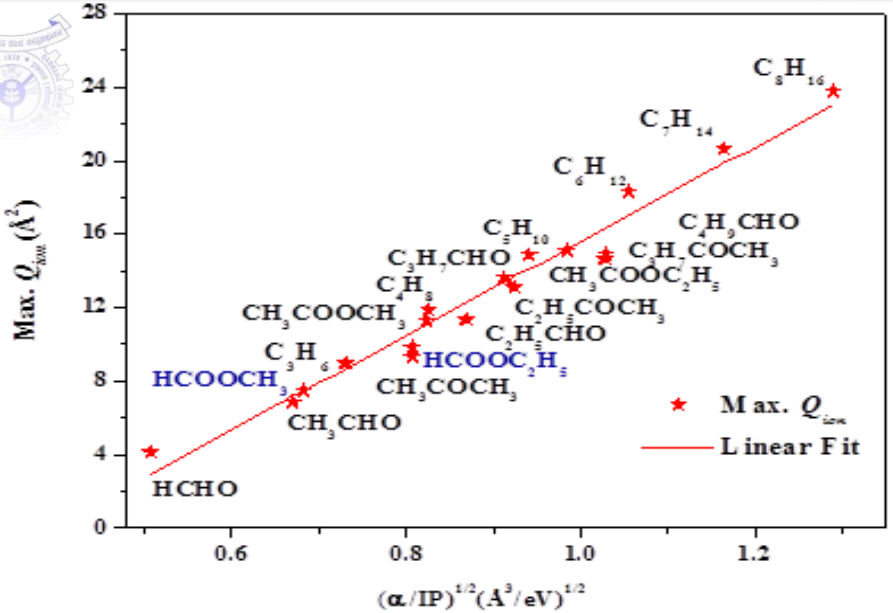


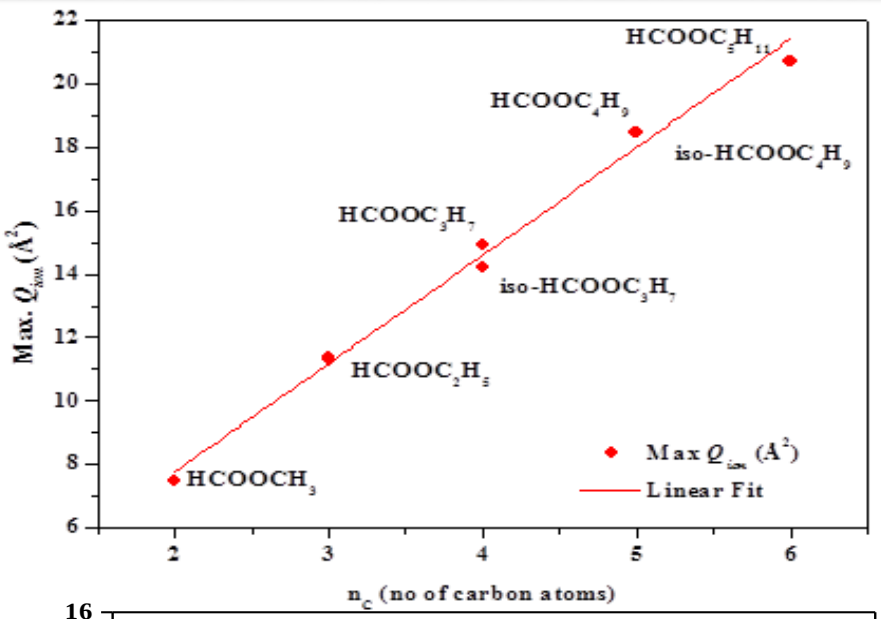


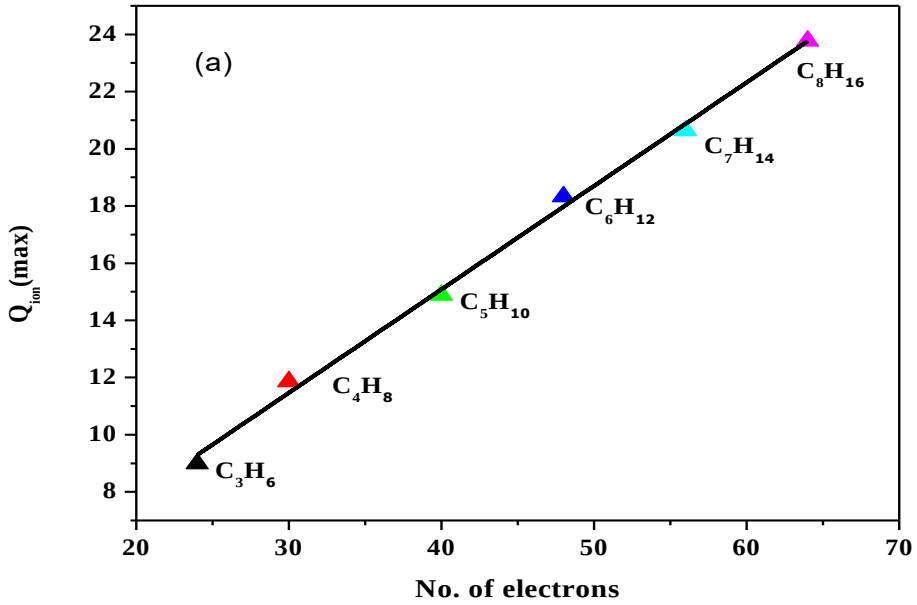


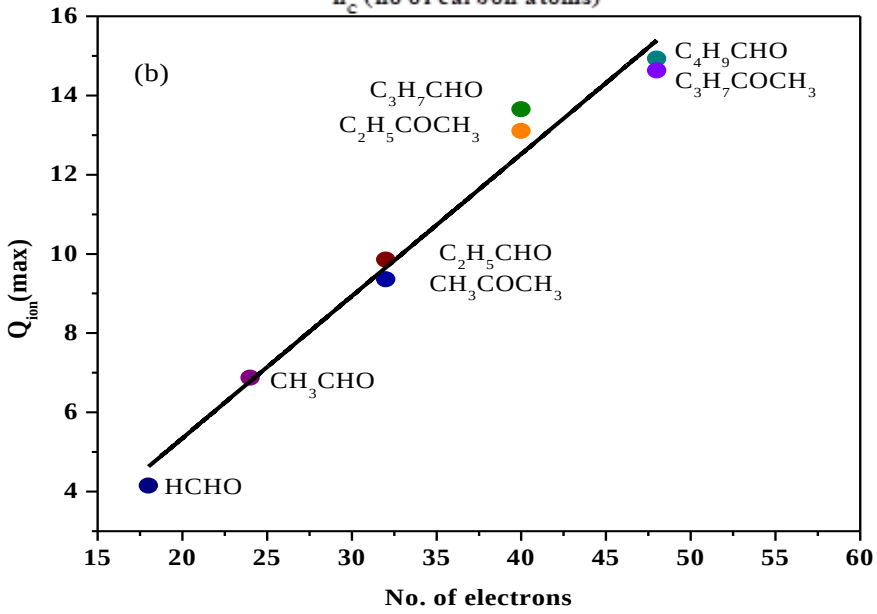


Uncertainty: Consistency check









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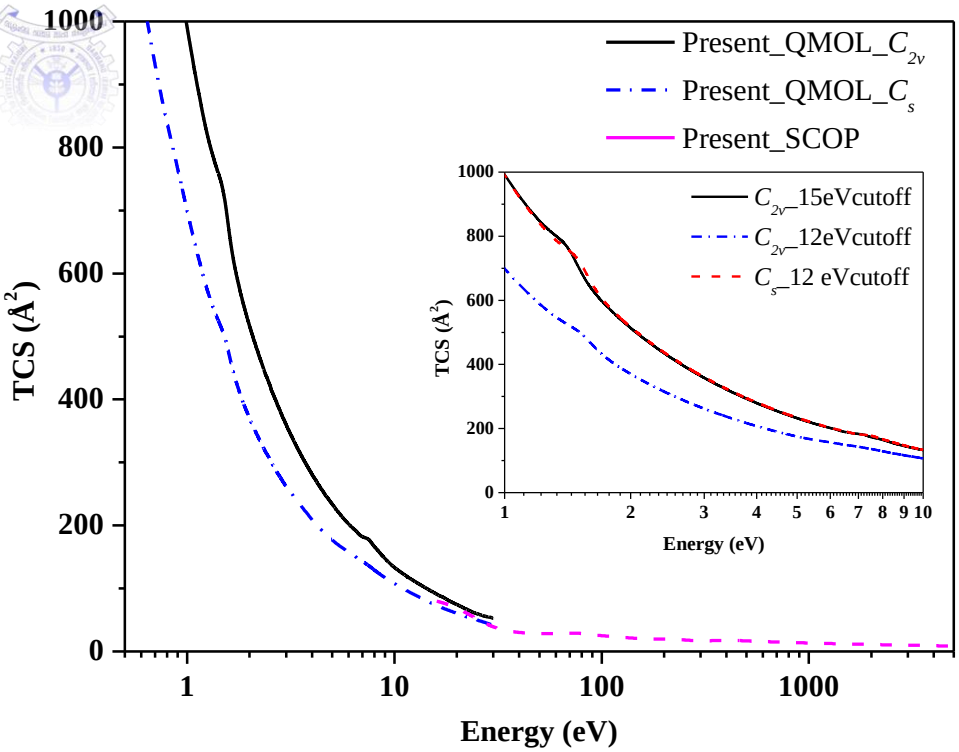
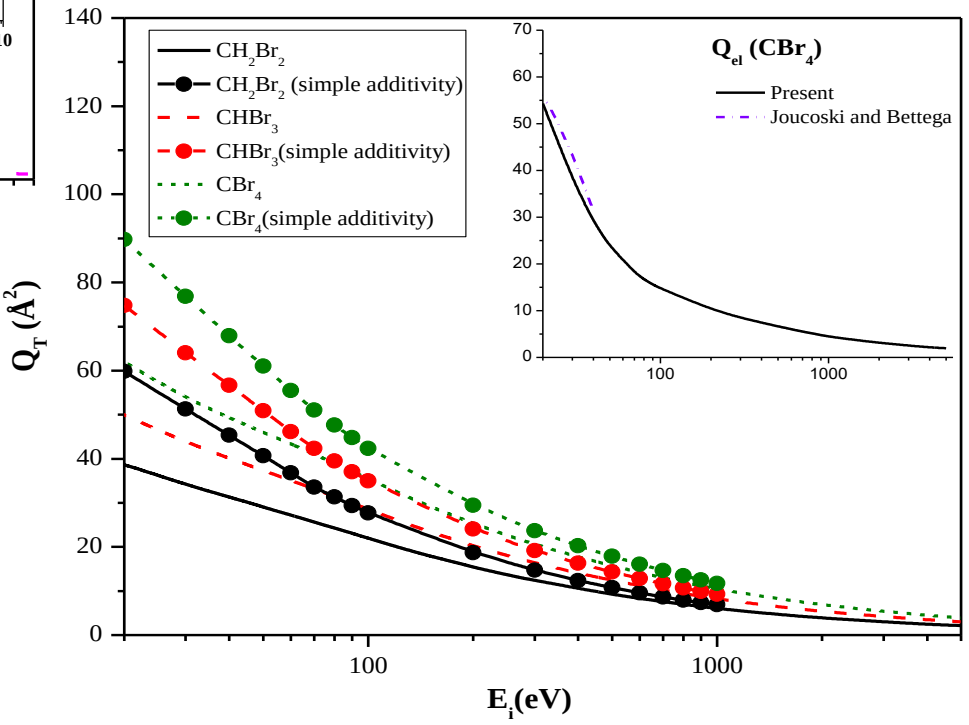
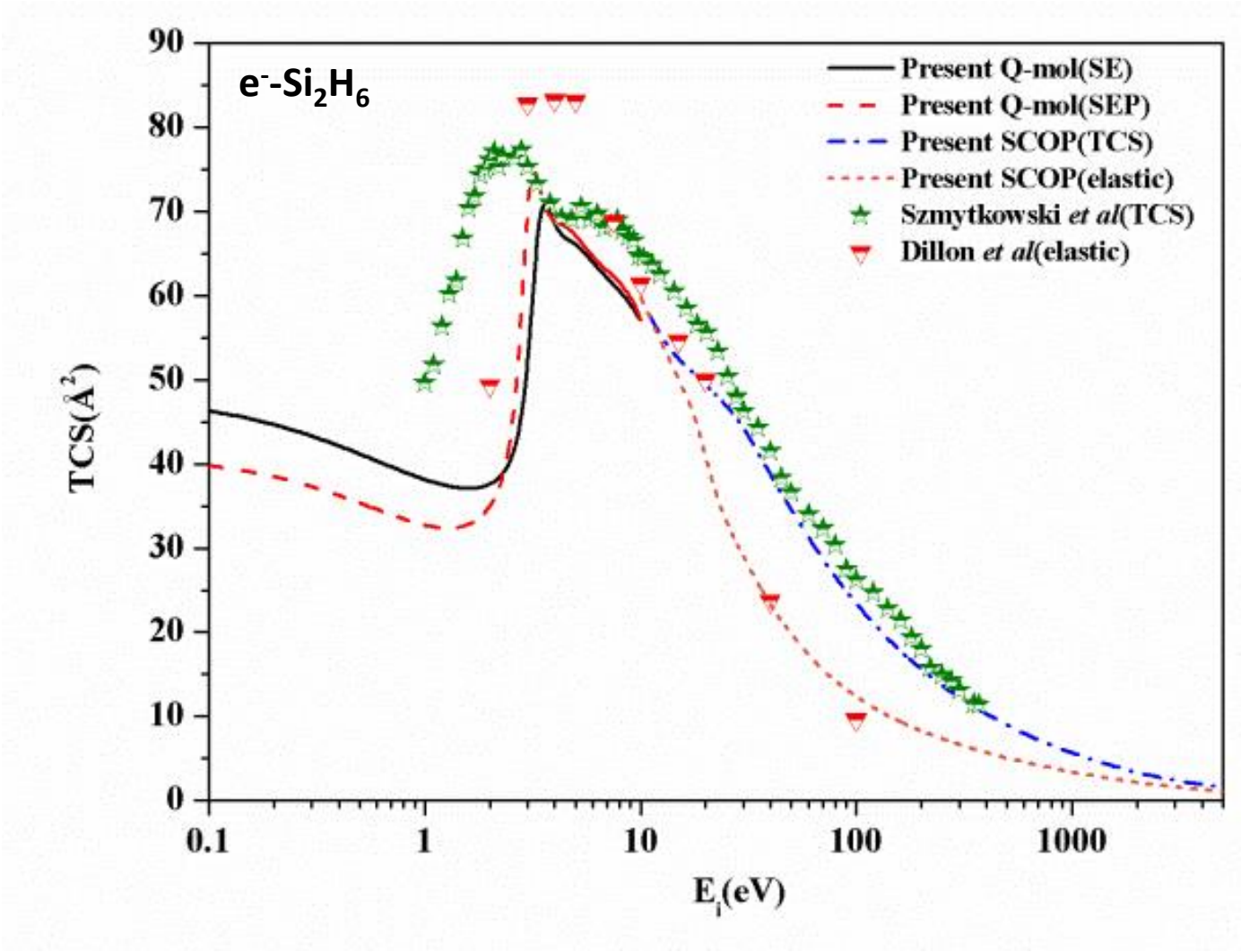
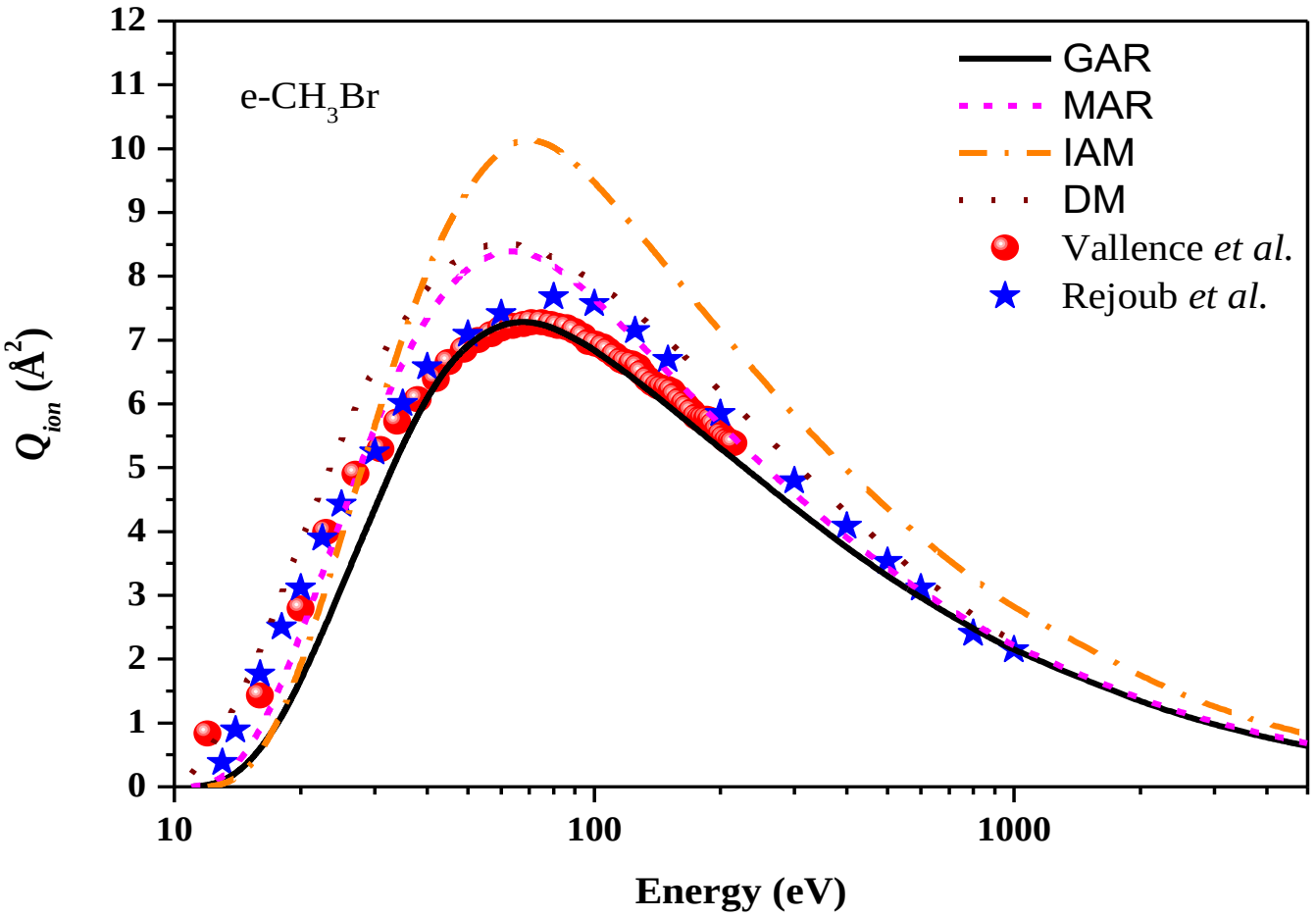




Uncertainty: Convergence check



Uncertainty: Convergence check



IAM: Independent Atom Model

MAR: Modified Additivity Rule

GAR: Group Additivity Rule

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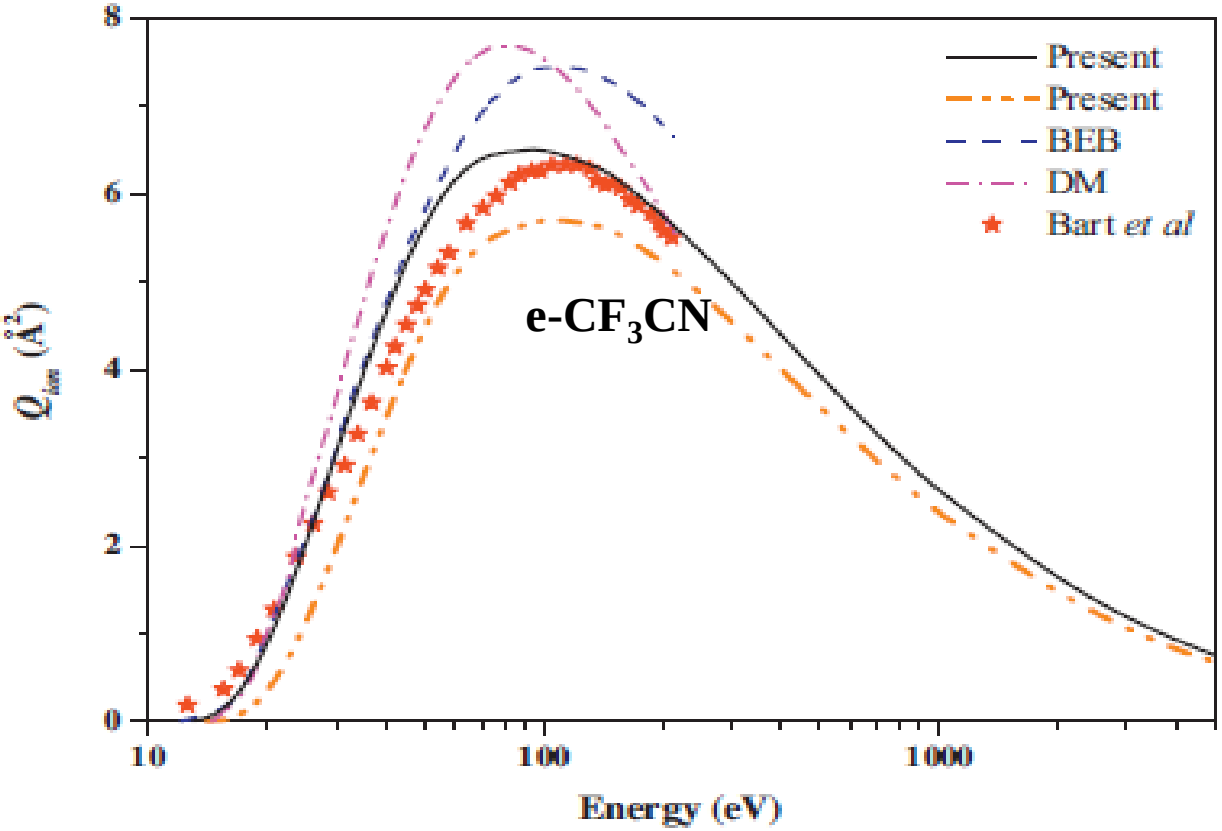
Sensitivity to ***Ionization Potential***

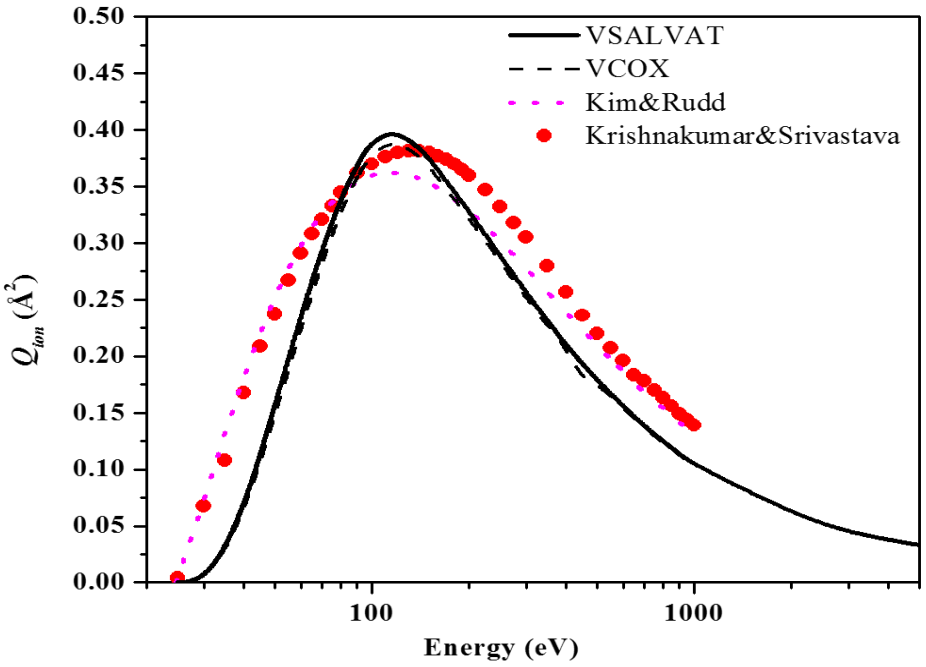
IP (CCCBDB) = 13.93 eV
IP (BEB threshold) = 12.11 eV

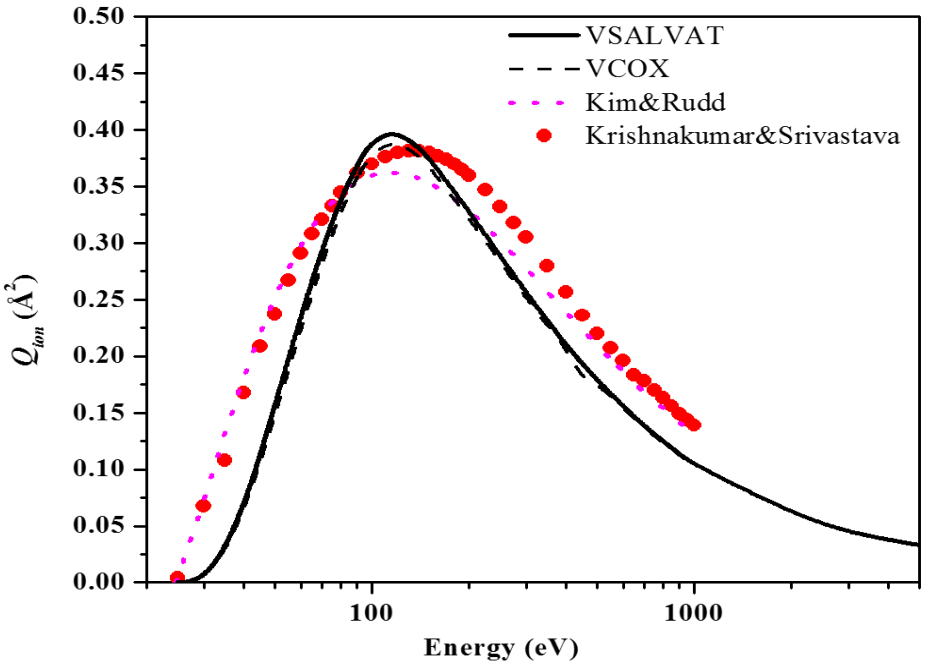


Deviation: ~14 %

Uncertainty: Sensitivity to input parameters

Sensitivity to ***Static Potential*** **(V_COX Vs V_SALVAT)**



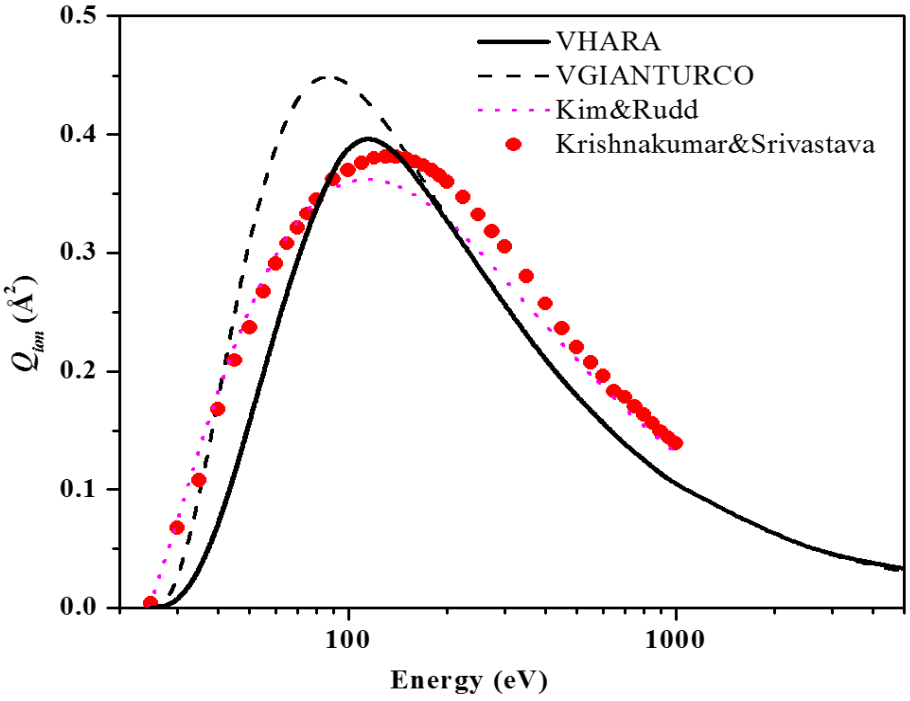


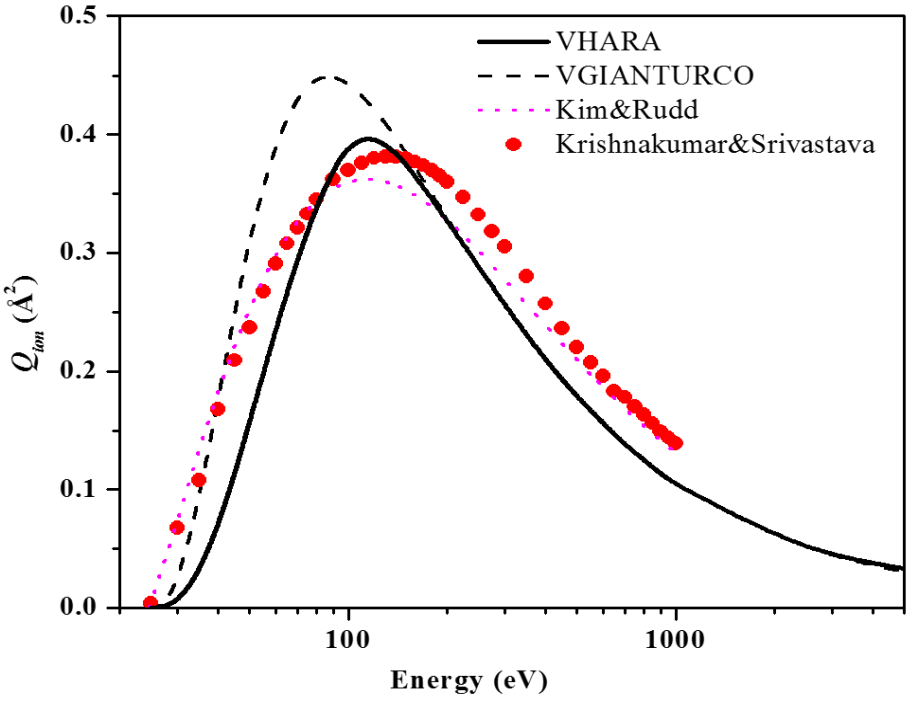
Deviation: ~2.29 %

Uncertainty: Sensitivity to input parameters

Sensitivity to ***Exchange Potential***

(V_HARA Vs V_GIANTURCO)

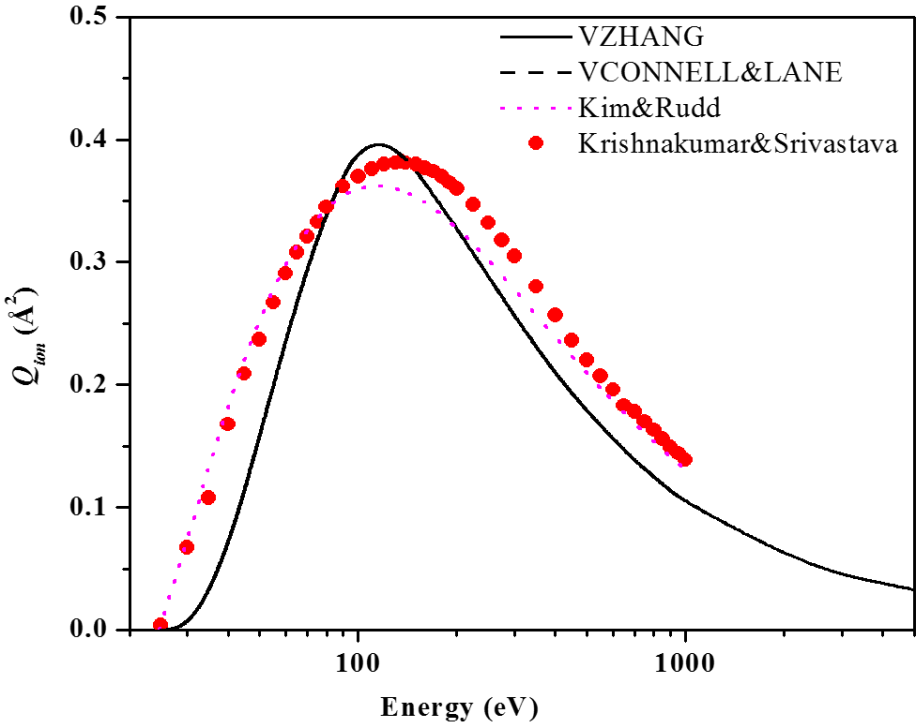


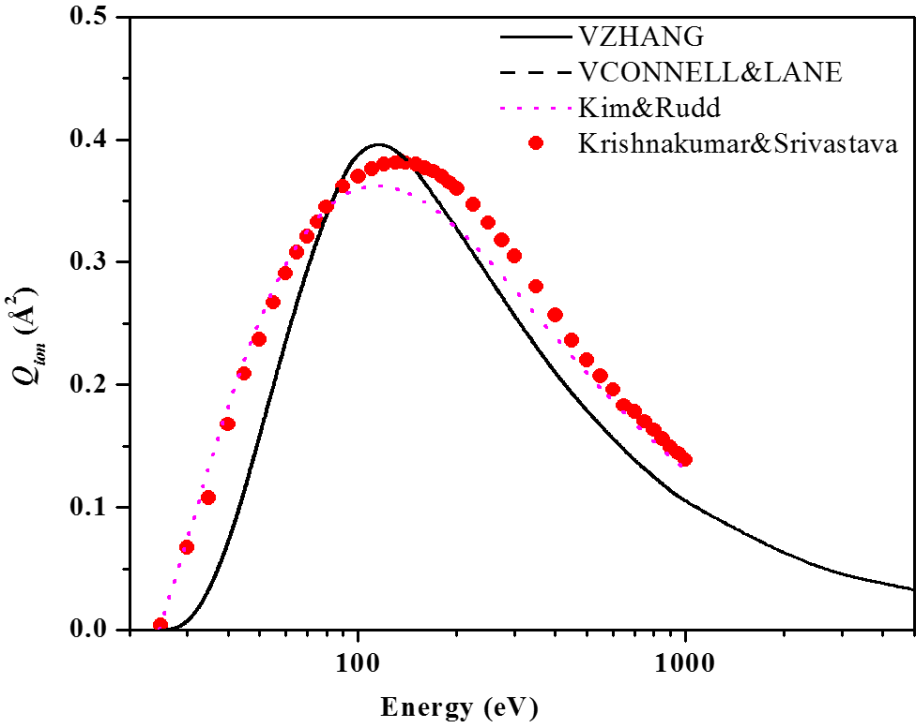


Deviation: ~13.2 %

Sensitivity to ***Polarization Potential***

(V_ZHANG Vs V_CONNELL&LANE)



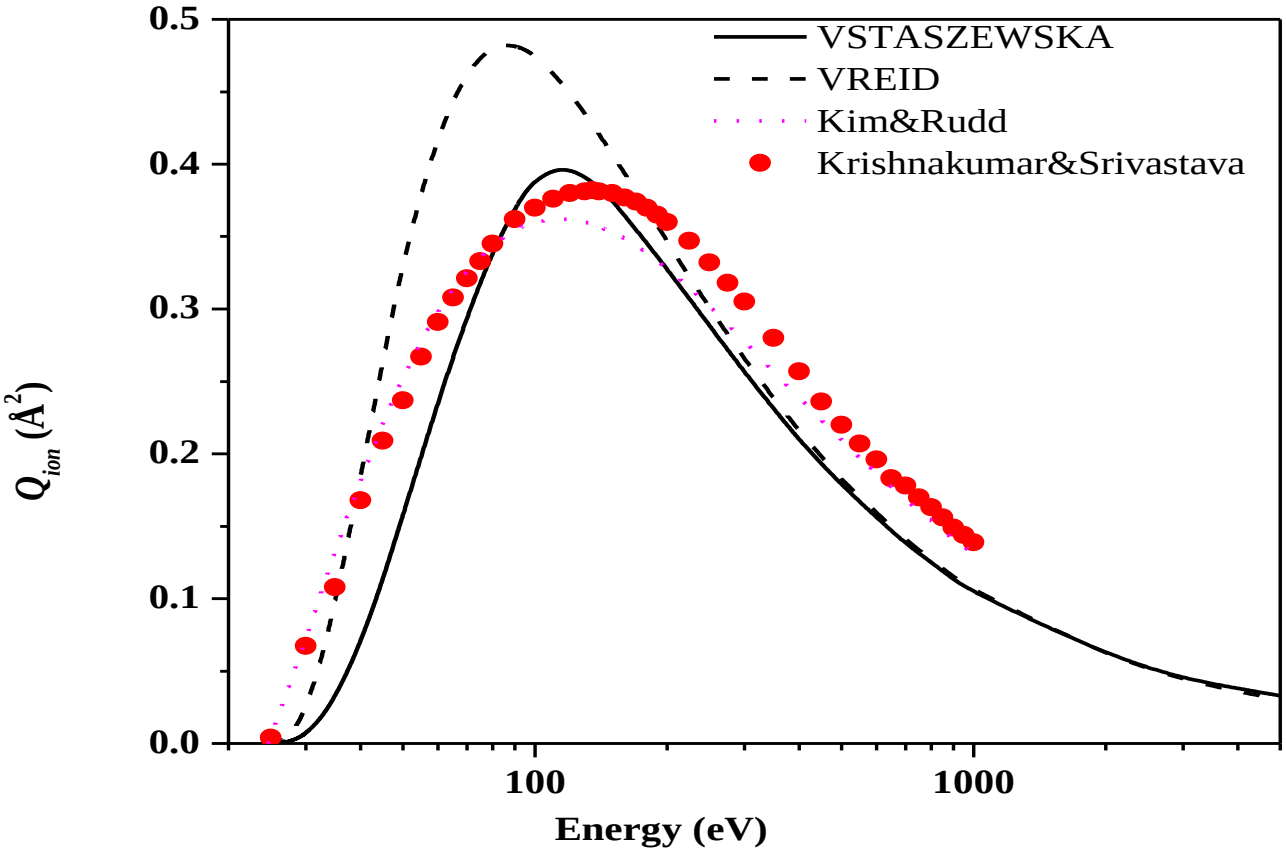


Deviation: ~0 %

Uncertainty estimation

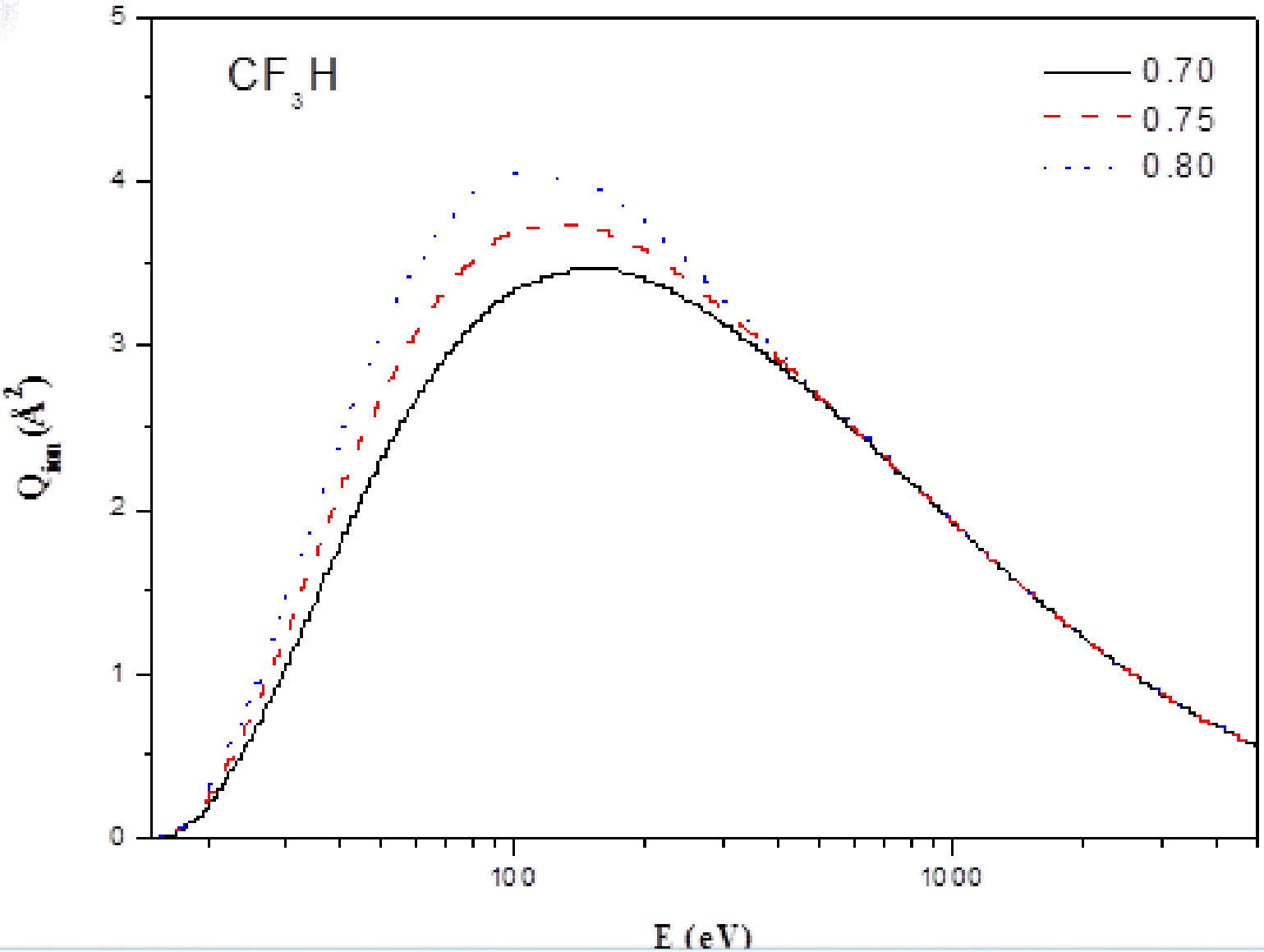
- Sensitivity to ***Absorption Potential***

(V_STASZEWSKA Vs V_REID)



Deviation: ~21.6 %

Uncertainty: Sensitivity to input parameters



Outline

- Need for cross section data
- Theoretical methodology & Sample Results
  - Electron Scattering
  - Positron Scattering
- **Uncertainty estimation**
  - Benchmarking Data
  - Consistency check
  - Convergence check
  - Sensitivity to input parameters
  - **Further plan**
- IAMDB

Uncertainty: Further plan

- Estimate uncertainties associated with cross section data.
- Develop a standard methodology???

Outline

- Need for cross section data
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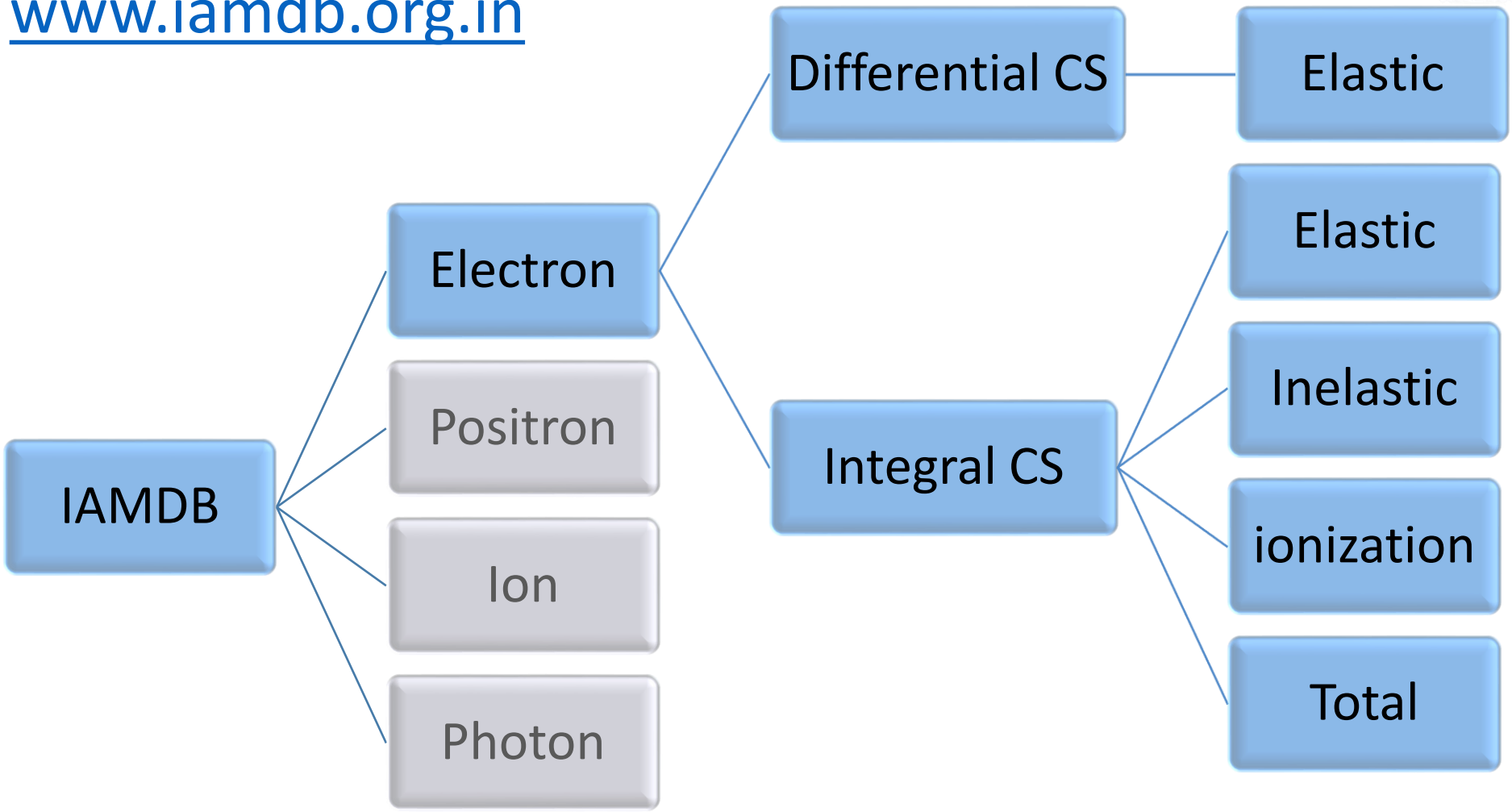
- **IAMDB**

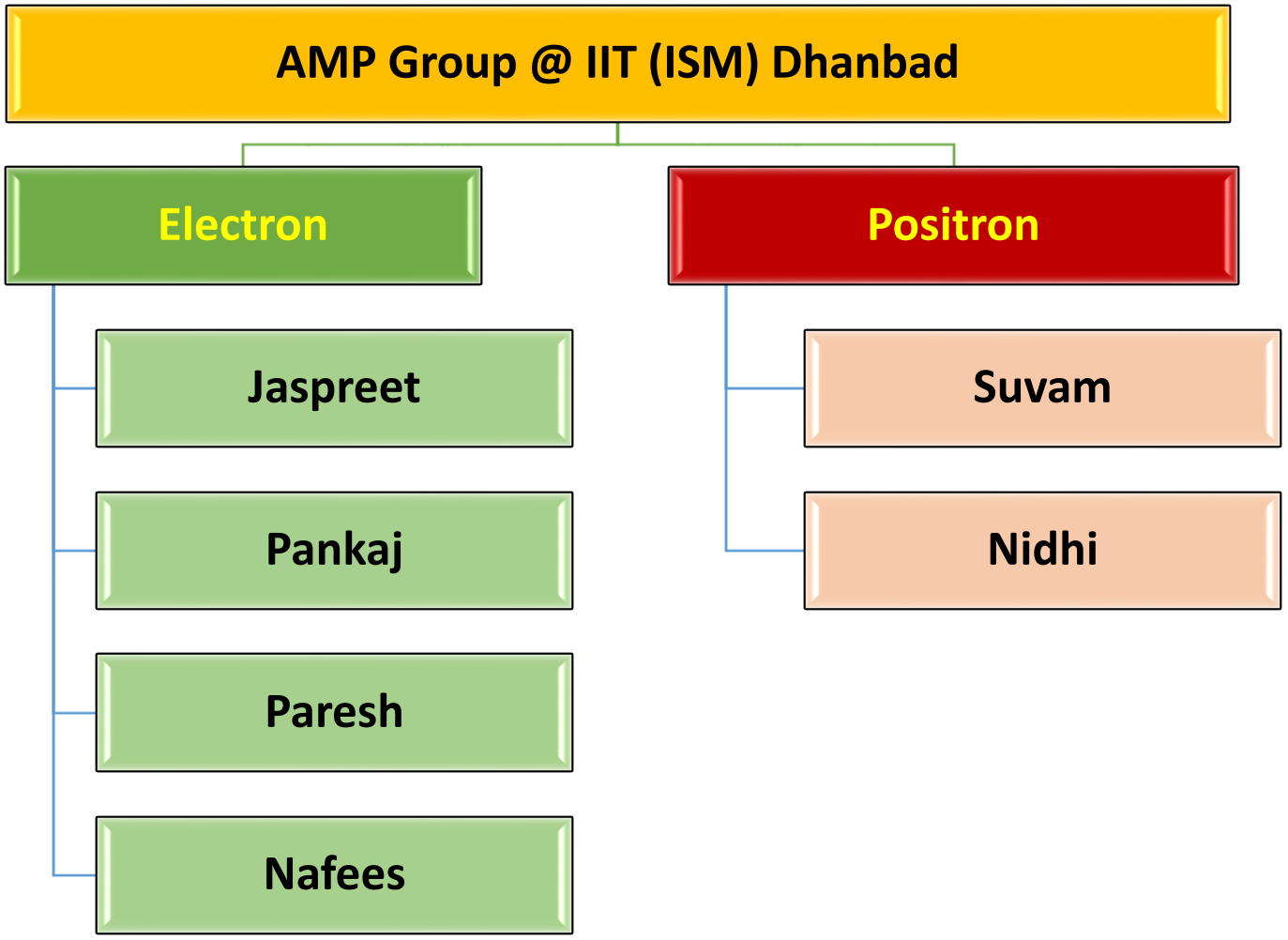
Indian Atomic & Molecular Database*

www.iamdb.org.in



* M.L. Dubernet, B. Antony, et al., J. Phys. B: At. Mol. Opt. Phys. **49** (2016) 074003.

Acknowledgement



Thank you