Electronic stopping power

current status of experimental data, theoretical and numerical descriptions

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Stopping Power Database, Nuclear Data Services, IAEA

Stopping power, interest

Electronic energy loss → excitations of the target electrons

Linear Stopping Power → $S = -\left\langle \frac{dE}{dl} \right\rangle$ Energy loss per unit path length ← eV/A

Stopping Cross Section → $SCS = \frac{S}{n}$ ← $\text{eV cm}^2/\text{atom}$, $\text{MeV cm}^2/\text{mg}$

n ← *target* density

$$SCS = \int dk\, d\omega\, \omega\, P(k,\omega)$$

Why the interest?

- **Knowledge of the basic physics** involved, the electronic structure of the target, the response of the electrons to the ion passage, interaction potential.
- **Applications**

Applications

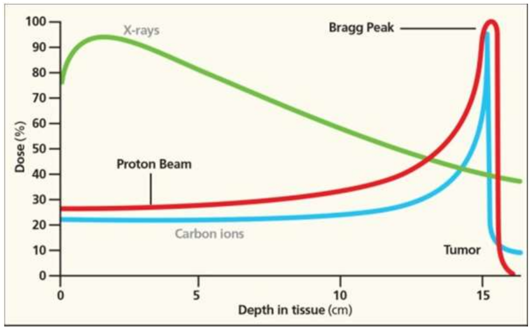
•**Ion beam analysis** of materials, nuclear research, fission fragment detectors,…., arqueology

•**Deposition ranges**

Hadron therapy for cancer

Detector of ions in satellites

MAPT - The Multi-purpose Active-target Particle Telescope



•**Ion implantation**

doping metal oxide semiconductors,

microelectronic devices and hard glasses

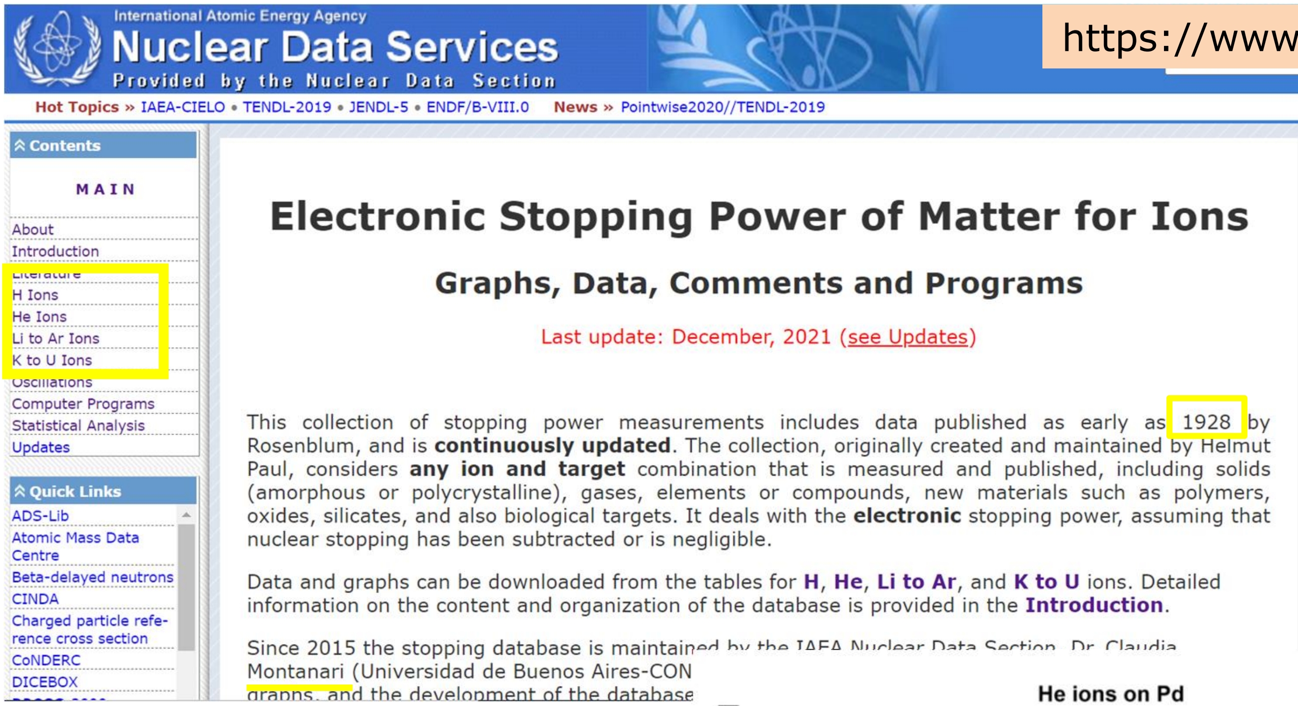
•**Material damage**

spacecraft shielding

Losses of molecular groups → $L= a\ (-dE/dx)^b$

Simulations include stopping values (most of them from SRIM)

Experimental state of art


International Atomic Energy Agency
Nuclear Data Services
Provided by the Nuclear Data Section

Hot Topics » IAEA-CIELO • TENDL-2019 • JENDL-5 • ENDF/B-VIII.0 News » Pointwise2020//TENDL-2019

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ADS-Lib
Atomic Mass Data Centre
Beta-delayed neutrons
CINDA
Charged particle reference cross section
CoNDERC
DICEBOX

Electronic Stopping Power of Matter for Ions

Graphs, Data, Comments and Programs

Last update: December, 2021 (see Updates)

This collection of stopping power measurements includes data published as early as 1928 by Rosenblum, and is **continuously updated**. The collection, originally created and maintained by Helmut Paul, considers **any ion and target** combination that is measured and published, including solids (amorphous or polycrystalline), gases, elements or compounds, new materials such as polymers, oxides, silicates, and also biological targets. It deals with the **electronic** stopping power, assuming that nuclear stopping has been subtracted or is negligible.

Data and graphs can be downloaded from the tables for **H**, **He**, **Li to Ar**, and **K to U** ions. Detailed information on the content and organization of the database is provided in the **Introduction**.

Since 2015 the stopping database is maintained by the IAEA Nuclear Data Section. Dr. Claudia Montanari (Universidad de Buenos Aires-CON... graphs, and the development of the database...

https://www-nds.iaea.org/stopping/

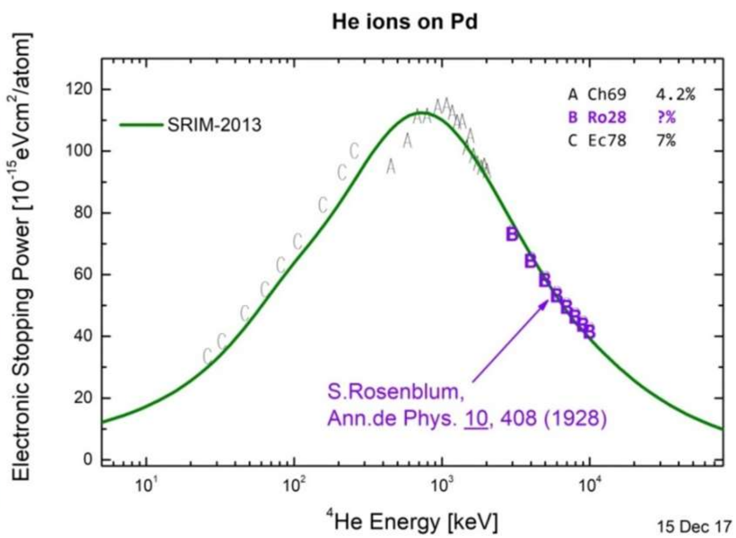
- **H. Paul,** 1990 - 2015
- **IAEA,** 2015 – present, C. Montanari
- **More than 90 years** of experimental data
- Around **4500 data sets, 59900 values,** 860 papers.
- All data is **open access** (tables)
- **Figures** for most (but not all...) systems

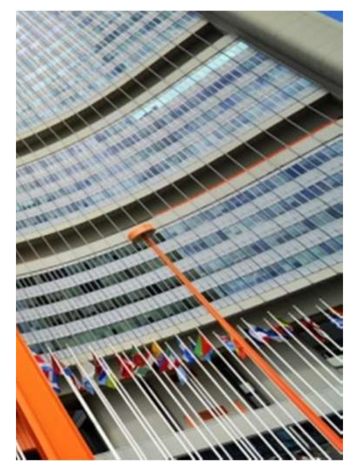
ANNALES DE PHYSIQUE

1928

RECHERCHES EXPÉRIMENTALES SUR LE PASSAGE DES RAYONS α A TRAVERS LA MATIÈRE

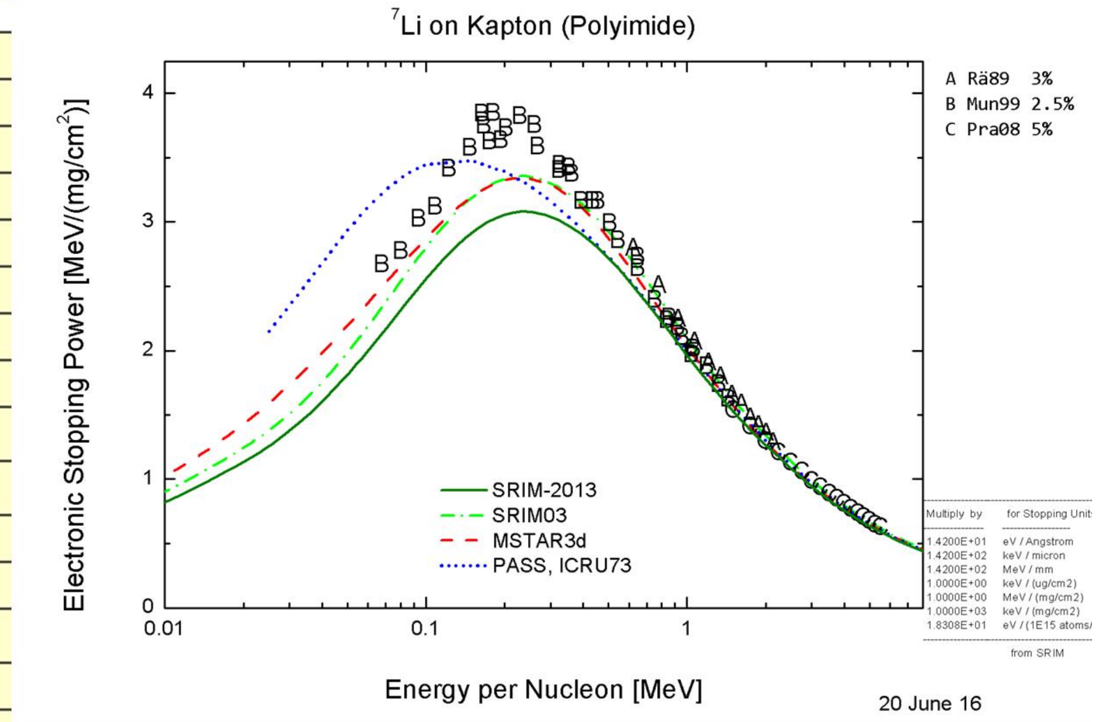
Par Salomon ROSENBLUM





At present, graphs are available for the following projectiles and ta

Projectiles	Target	Graphs:	
$_3$Li ions	Ag	Click here	
	Air	Click here	
	Al	Click here	
	Ar	Click here	
	Au	Click here	
	B	Click here	
	C	Click here	
	CH_4	Click here	
	CO_2	Click here	
	Cu	Click here	
	Gd	Click here	
	H_2	Click here	
	He	Click here	
	Lu	Click here	
	Kapton (polyimide)	Click here	Complete data table (txt file), origin figure
	Mylar	Click here	
	N2	Click here	
	Ne	Click here	*D*
	Ni	Click here	*T*
	Pd	Click here	
	Polycarbonate	Click here	
	Polypropylene	Click here	
	Si	Click here	T C
	SiO2	Click here	
	Ta	Click here	

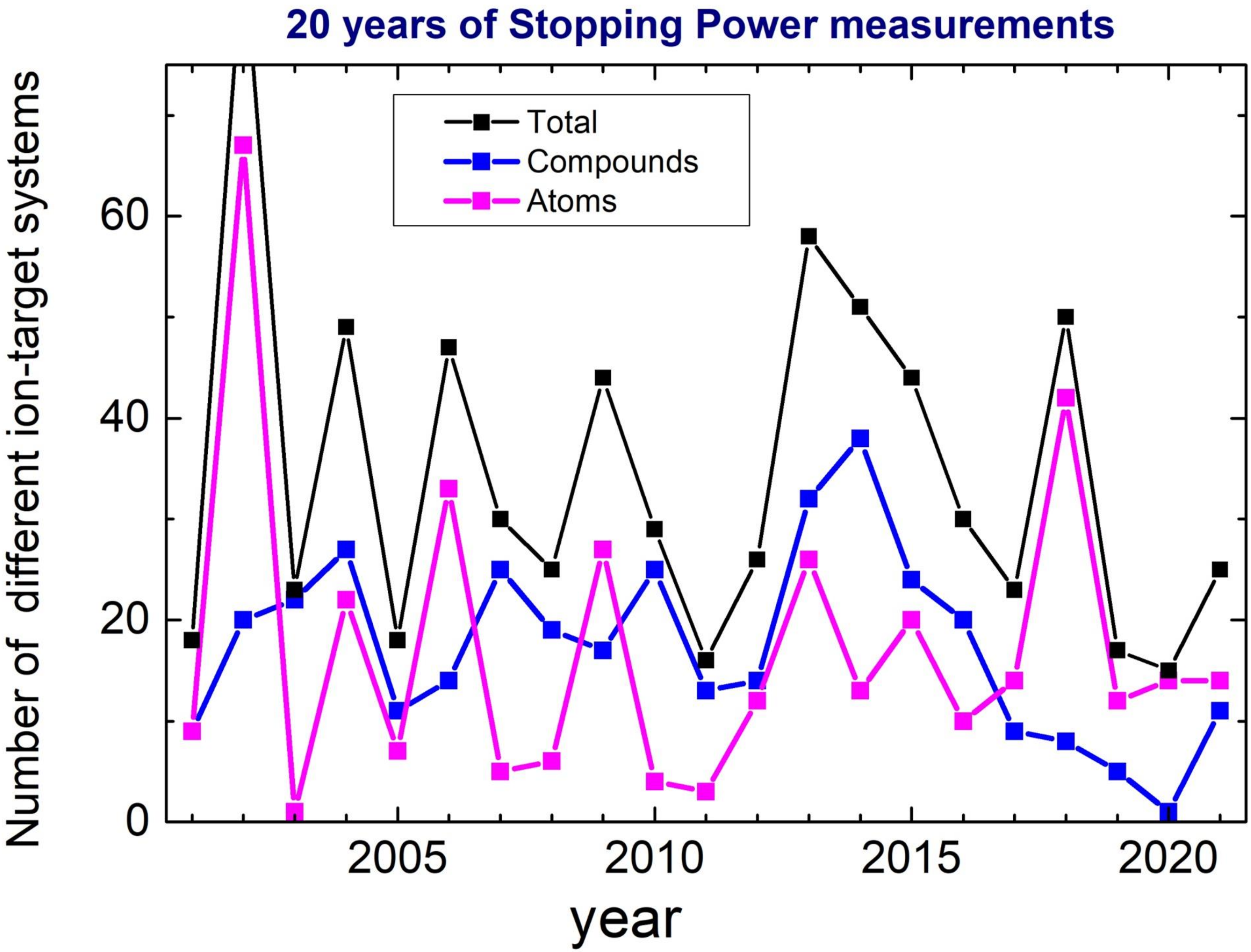


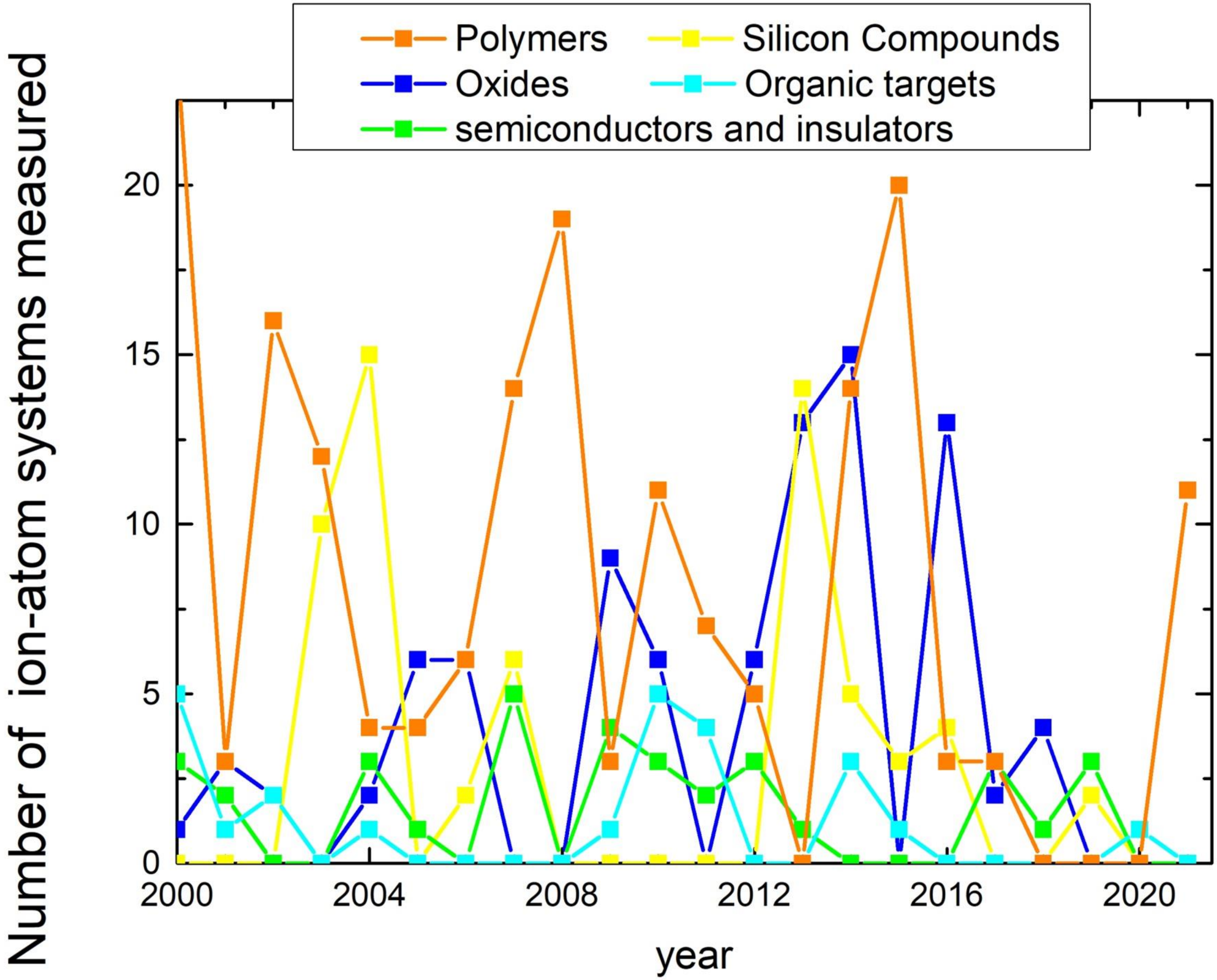
7LiKapto: Bloc de notas

Archivo Edición Formato Ver Ayuda

2.14	1.27	A	Rä89	J.Räisänen and E.Rauhala, Radiation Eff. and Def. in Solids 108,21 (1989)
2.008571	1.34	A	--	
1.878571	1.4	A	--	--
1.747143	1.46	A	--	--
1.61	1.57	A	--	--
1.48	1.64	A	--	--
1.342857	1.78	A	--	--
1.207143	1.89	A	--	--
1.067143	2.05	A	--	--
0.9242857	2.23	A	--	--
0.7757143	2.49	A	--	--
0.6214285	2.78	A	--	--
0.0676	2.652	B	Mun99	F.Munnik,K.Väkeväinen,J.Räisänen,U.Wätjen, J.Appl.Phys. 86,3934 (1999)
0.0801	2.758	B	--	
0.0937	3.009	B	--	--
0.1081429	3.102	B	--	--
0.1227143	3.395	B	--	--
0.1472857	3.559	B	--	--
0.164	3.827	B	--	--
0.1665714	3.73	B	--	--
0.1754286	3.61	B	--	--
0.1814286	3.831	B	--	--
0.1932857	3.62	B	--	--
0.2021429	3.712	B	--	--
0.2287143	3.805	B	--	--
0.2602857	3.737	B	--	--
0.2668571	3.569	B	--	--

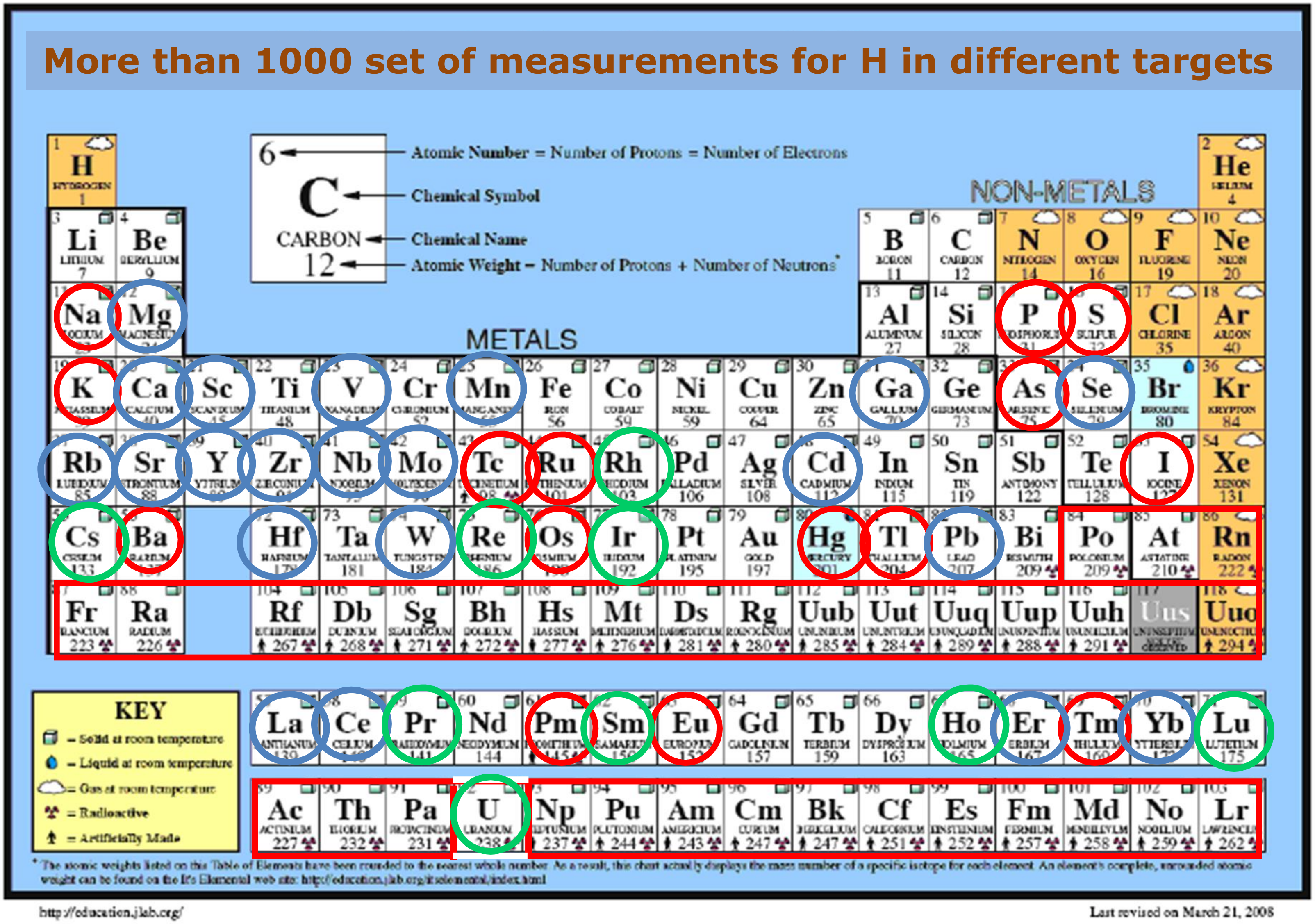
Experimental facilities, since 2010


20 years of Stopping Power measurements
Total
Compounds
Atoms
Number of different ion-target systems
year
0
20
40
60
2005
2010
2015
2020


Polymers
Silicon Compounds
Oxides
Organic targets
semiconductors and insulators
Number of ion-atom systems measured
year
0
5
10
15
20
2000
2004
2008
2012
2016
2020

H ions

Updated 2021



no data available

Only one set of data

no data at low energies

Stopping models

Theoretical schemes covering a wide energy range.

Scheme	Code	Target	Starting at	Domain	
Binary theory	PASS	Atom	Bohr	High v downward	Sigmund
PCA/UCA	CasP	Atom	Bethe-Bloch	High v downward	Grande Schiwietz
TCS-EFSR	HISTOP	Fermi gas	Quantal	Low v upward	Arista
SLPA		Atom/molec	Quantal	High v downward	Montanari Miraglia
MELF-GOS		Atom/molec	*Exp ELF*	*High v downward*	Abril García Molina
CDW-EIS		Atoms/Gases	*Quantal*	*High v downward*	Rivarola Miraglia
TD-DFT		Fermi gas	*Quantal*	*Low v*	Echenique Correa
TD-END		Atoms/molec	*Quantal*	*Low v*	Cabrera-Trujill Sabin

online, 2021

Ref: Sigmund & Schinner, NIM 382 (2016) 15-25

Stopping models

Theoretical schemes covering a wide energy range.

online, 2021

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SLPA		Atom/molec	Quantal	High v downward	Montanari Miraglia
					Abril

Open subjects, difficulties, challenges:

- Heavy projectiles, Li to U
- Multielectronic targets, 4f electrones, lanthanides and heavy transition metals
- Complex molecules →biological interest, plastics, oxides

TD-END		Atoms/molec	*Quantal*	*Low v*	Cabrera-Trujill Sabin

Ref: Sigmund & Schinner, NIM 382 (2016) 15-25

Stopping reliable values, semiempirical and empirical codes

Multiperpose simulations need reliable stopping values

SRIM The Stopping and Range of Ions in Matter, by Ziegler **(2013)**

Geant 4, Monte Carlo simulations, TALYS 1.6; include SRIM

Semi-empirical

MSTAR for Li to Ar in solids and gases, by H. Paul and A. Schinner (2003)

empirical

ASTAR, PSTAR for protons and alphas in different targets, by Berger, NIST (1992)

https://www-nds.iaea.org/stopping/stopping_prog.html

ICRU Reports (*International Commission on Radiation Units & Measurements)*

→ ICRU 37 (1984) for electrons and positrons
→ ICRU 49 (1993) for H and He
→ ICRU 73 (2005) for Li to Ar

MACHINE LEARNING:

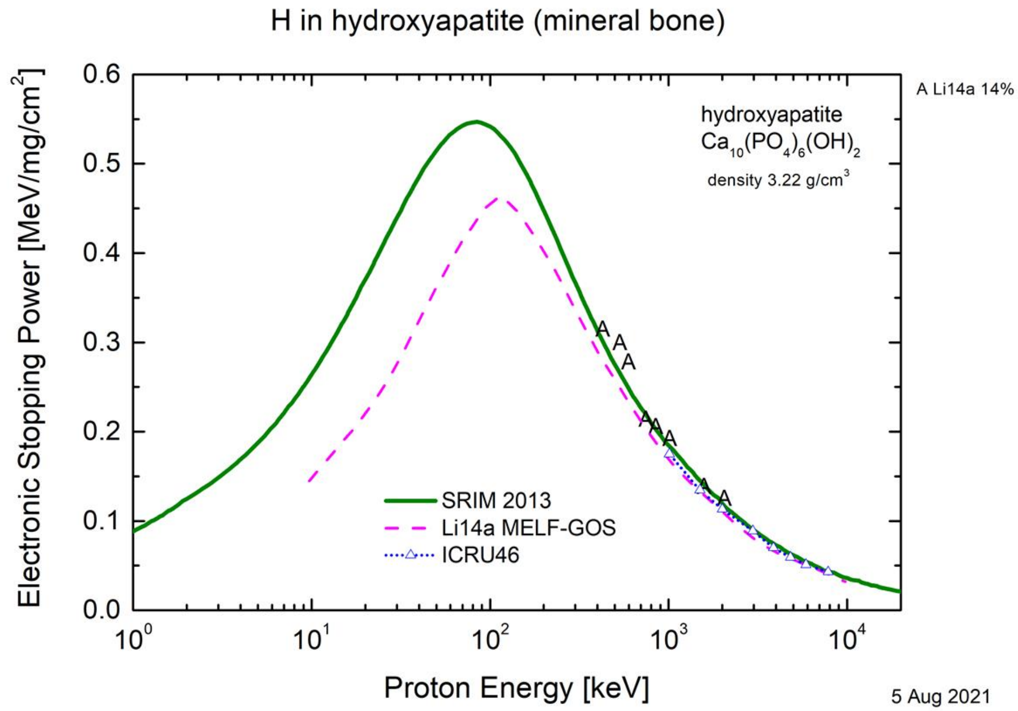
ML Parfitt-Jackman, NIMB 478 (2020) 21-33

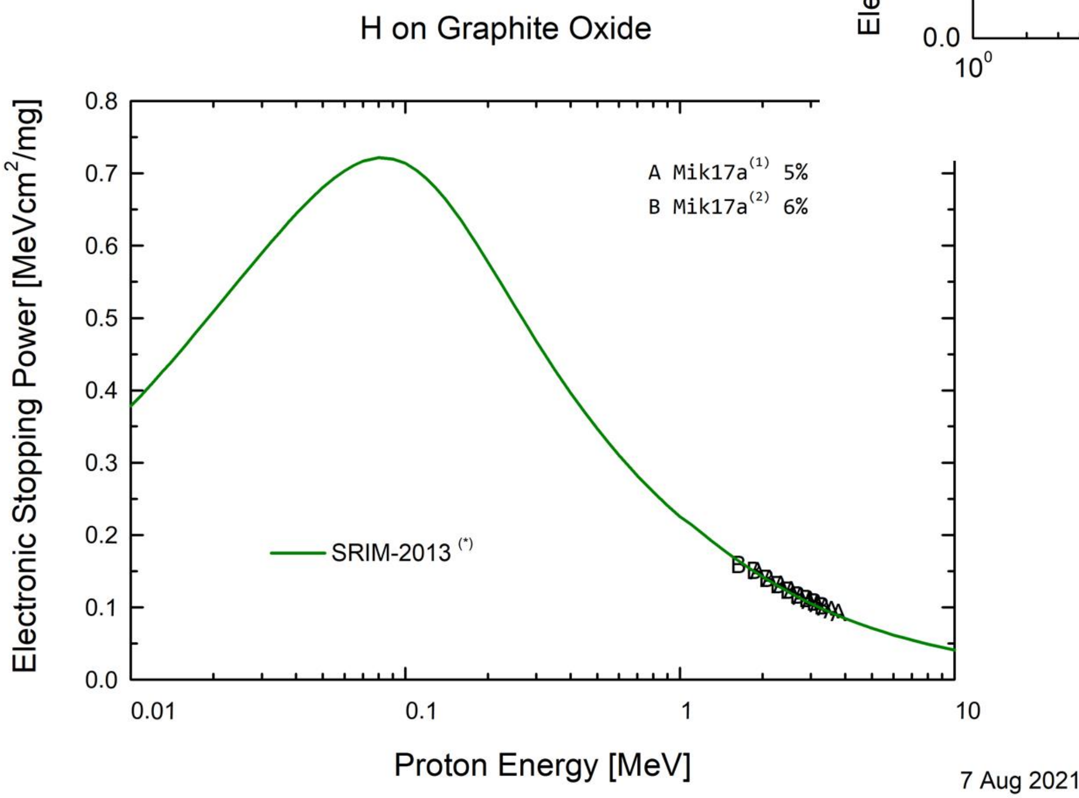
ML/deep neural network Mitnik et al (2022)

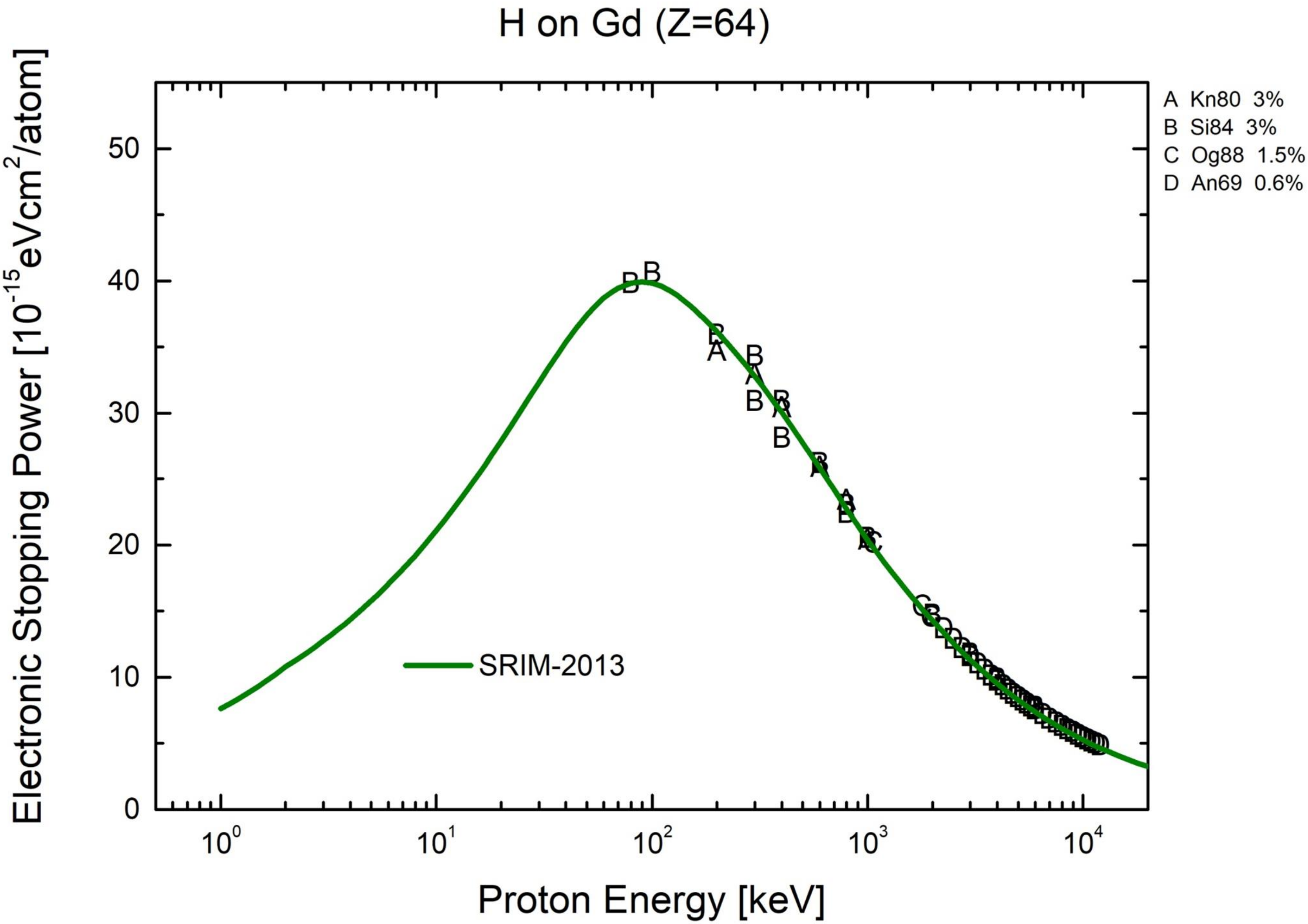
Experimental values from IAEA stopping database

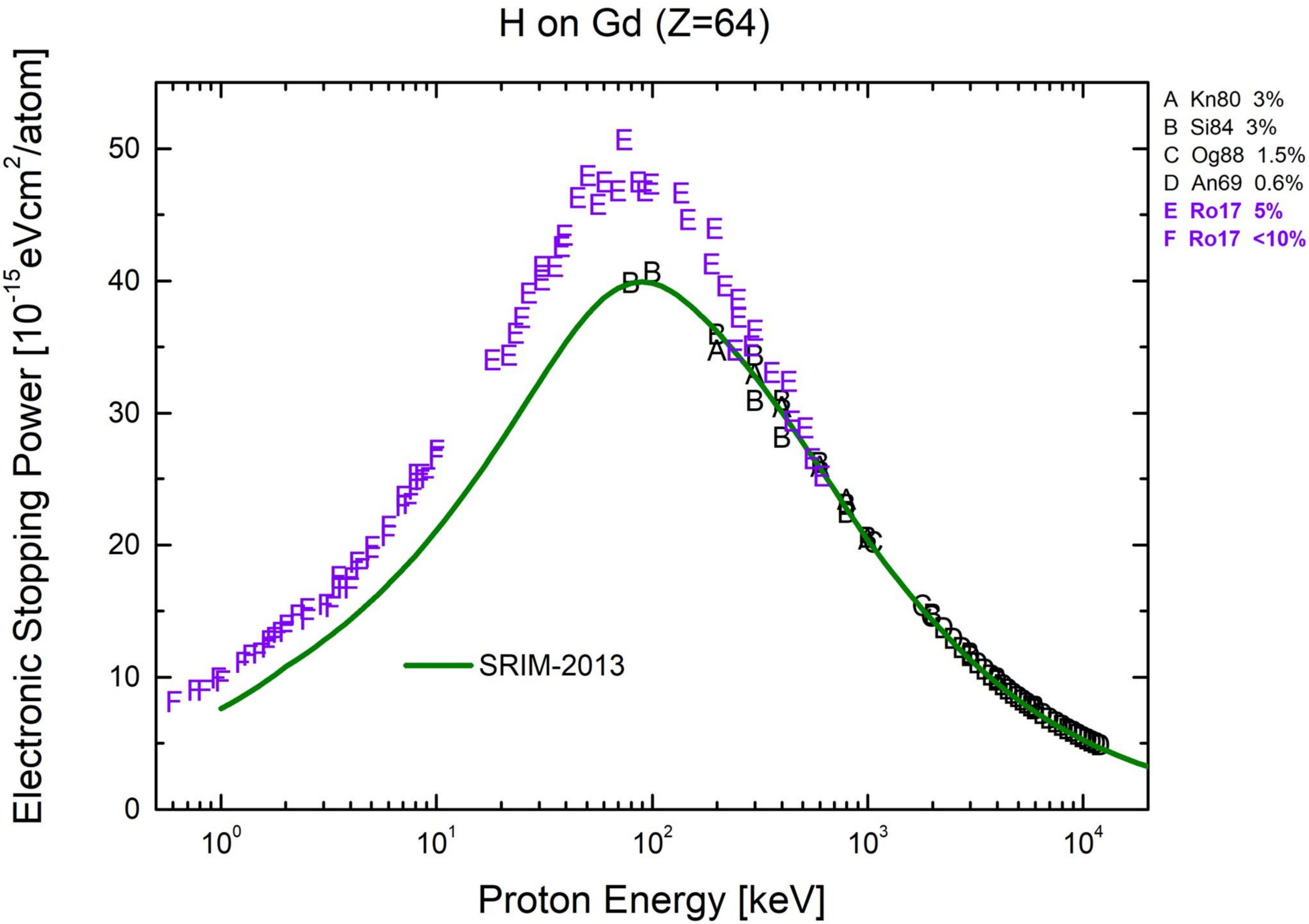
SRIM

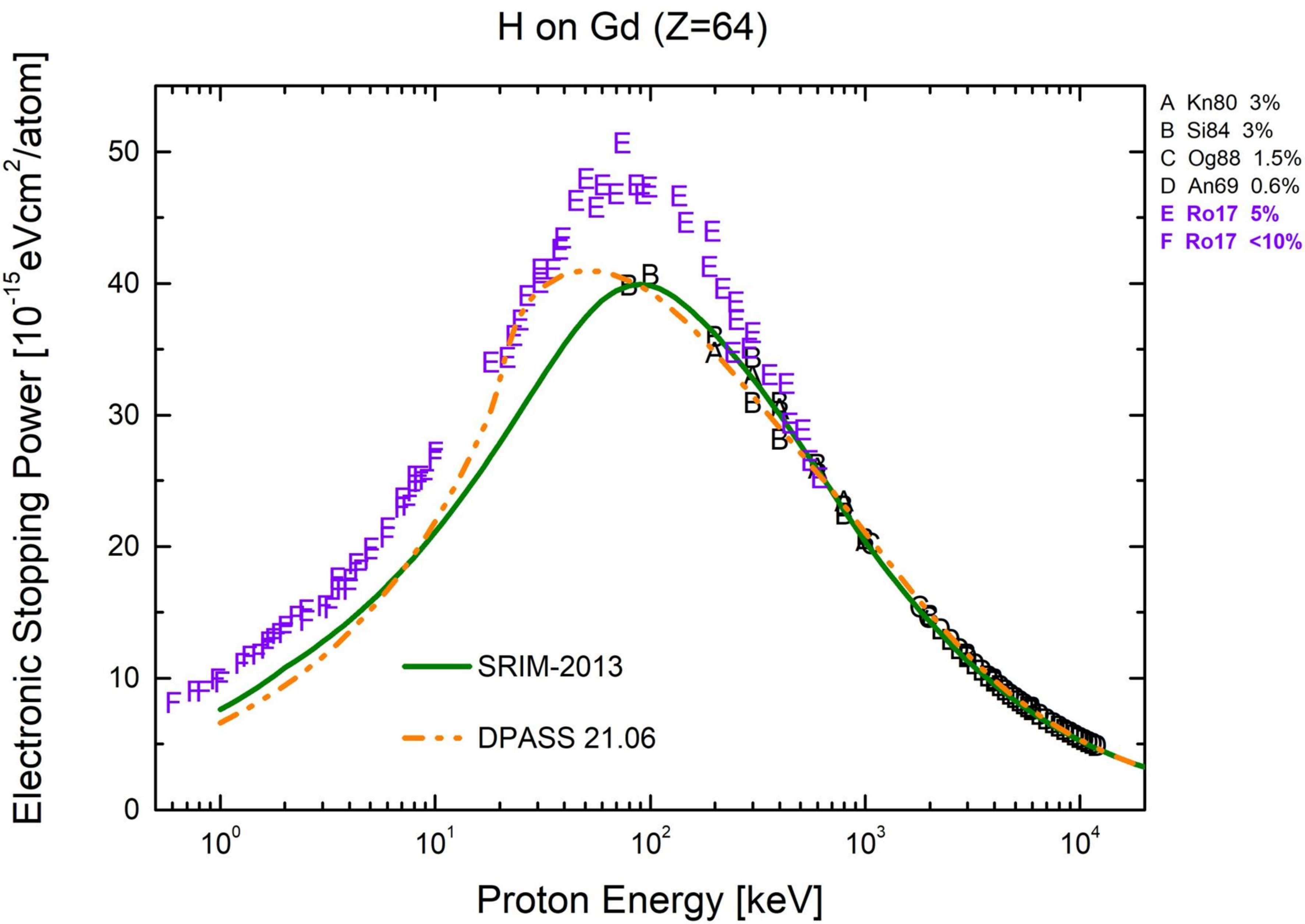
Experimental measurements after 2013. Good agreement

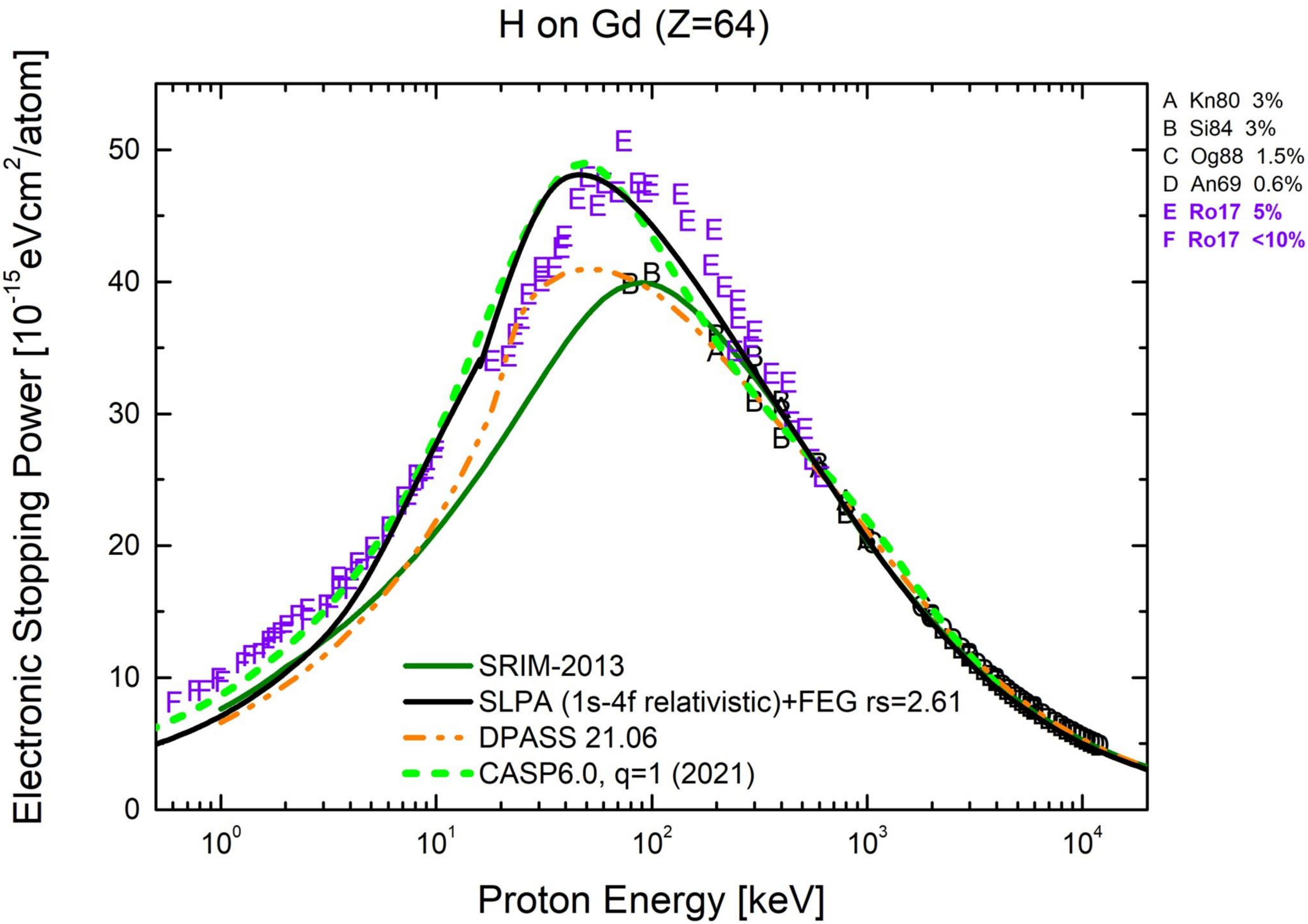





H on Gd (Z=64)
Electronic Stopping Power [10^-15 eVcm^2/atom]
Proton Energy [keV]
A Kn80 3%
B Si84 3%
C Og88 1.5%
D An69 0.6%
SRIM-2013
0
10
20
30
40
50
10^0
10^1
10^2
10^3
10^4


H on Gd (Z=64)
Electronic Stopping Power [10^-15 eVcm^2/atom]
Proton Energy [keV]
A Kn80 3%
B Si84 3%
C Og88 1.5%
D An69 0.6%
E Ro17 5%
F Ro17 <10%
SRIM-2013

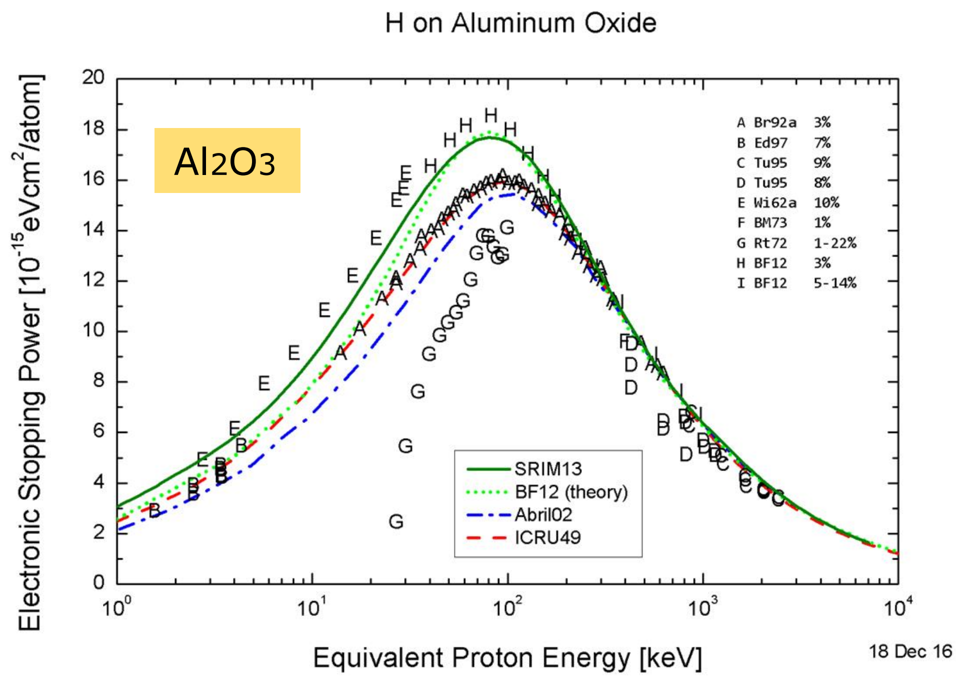

H on Gd (Z=64)
Electronic Stopping Power [10^-15 eVcm^2/atom]
Proton Energy [keV]
A Kn80 3%
B Si84 3%
C Og88 1.5%
D An69 0.6%
E Ro17 5%
F Ro17 <10%
SRIM-2013
DPASS 21.06



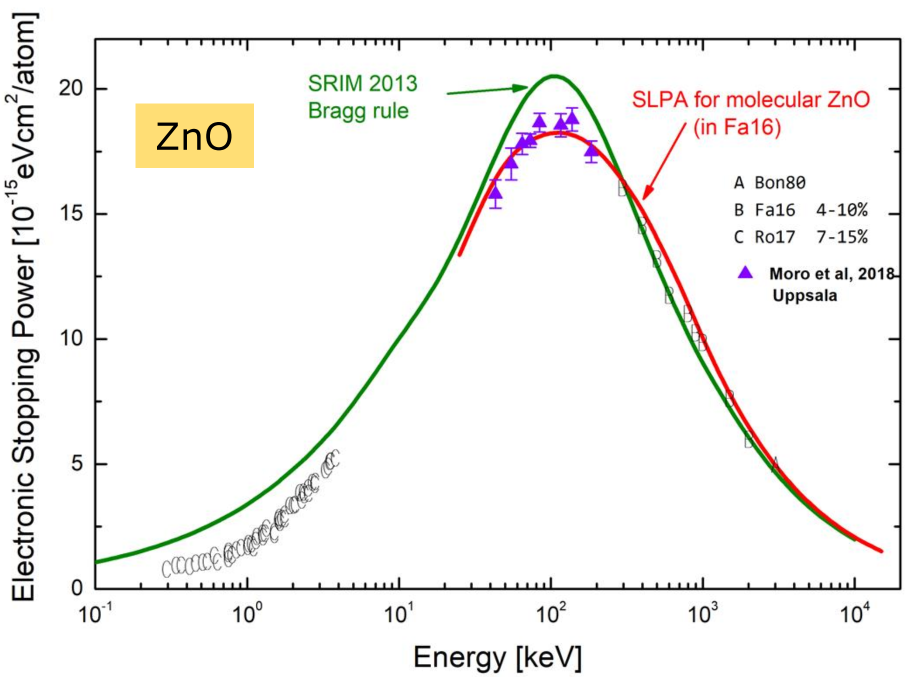
H on Gd (Z=64)
Electronic Stopping Power [10^{-15}eVcm^2/atom]
Proton Energy [keV]
0
10
20
30
40
50
10^0
10^1
10^2
10^3
10^4
A Kn80 3%
B Si84 3%
C Og88 1.5%
D An69 0.6%
E Ro17 5%
F Ro17 <10%
SRIM-2013
SLPA (1s-4f relativistic)+FEG rs=2.61
DPASS 21.06
CASP6.0, q=1 (2021)

Compounds

$2xAl+3xO$



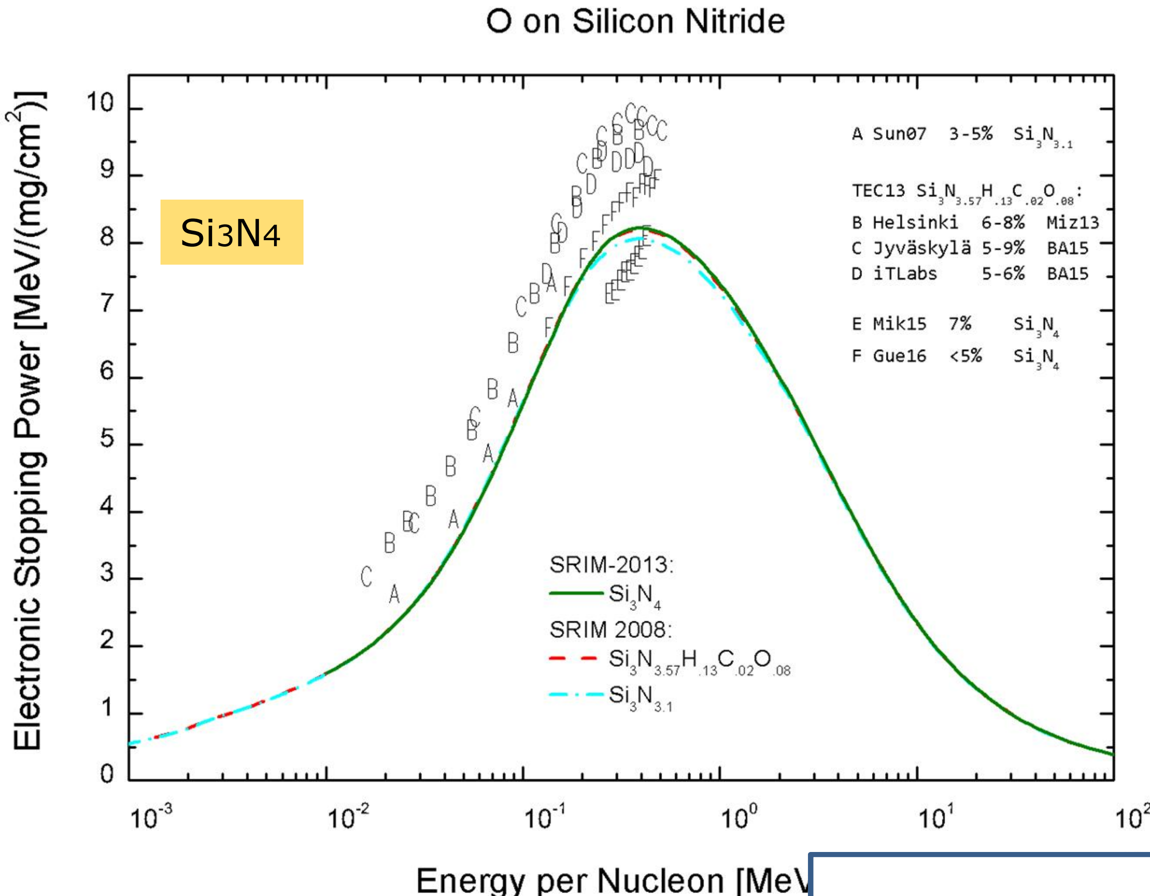
$Zn+ O$



SRIM code has an option for compound correction.

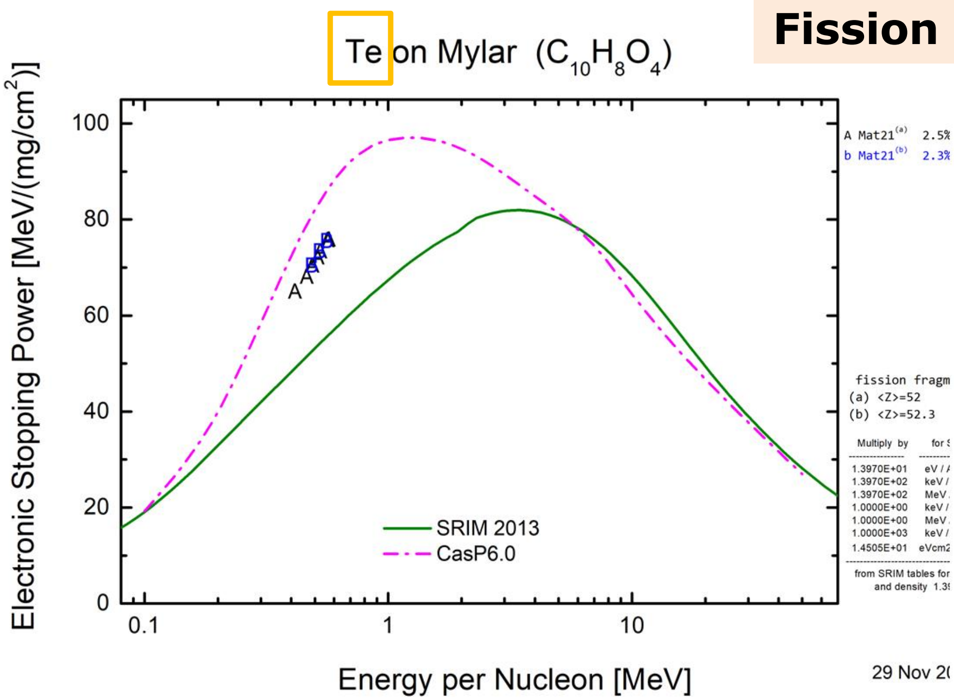
It separates core and bond contributions and alters the stopping for the bonding electrons based on the bonds found in the compound.

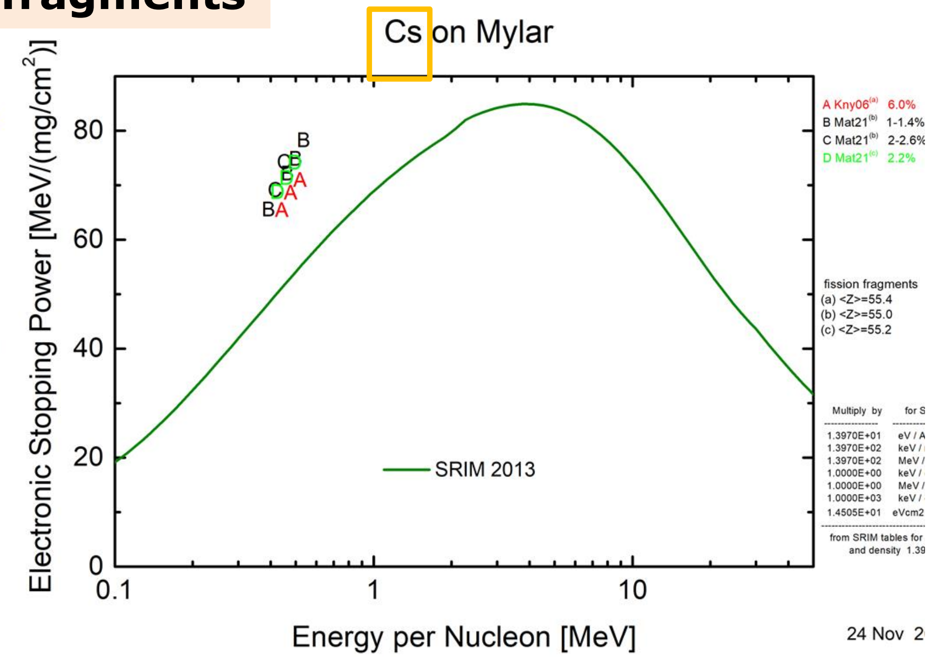
Compounds

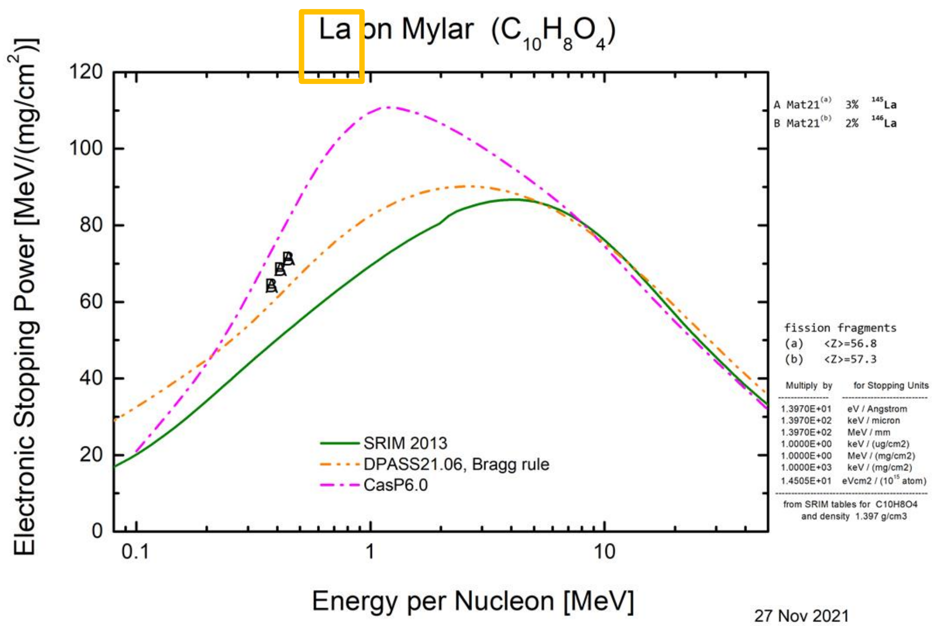


- high-melting-point 1900°C
- relatively chemically inert
- automobile industry (diesel engines, turbochargers, etc)
- Si3N4 bearings in engines of NASA's Space Shuttle.

Fission fragments

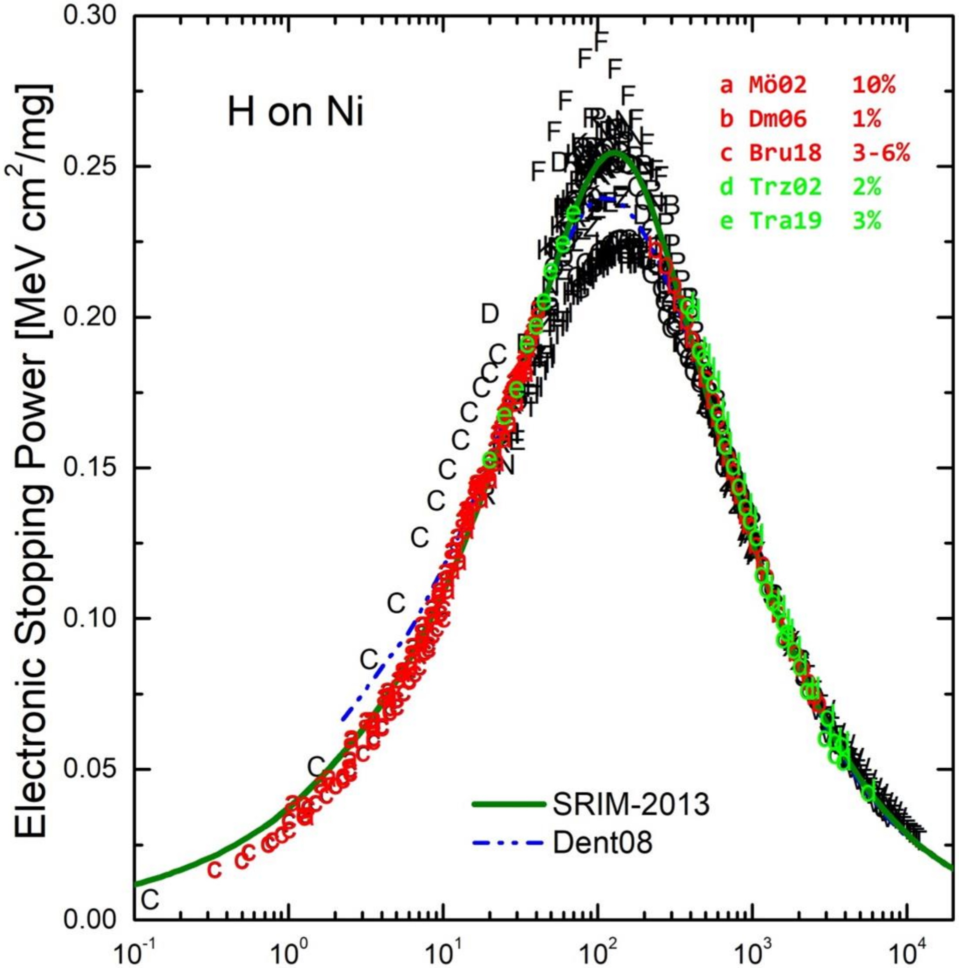




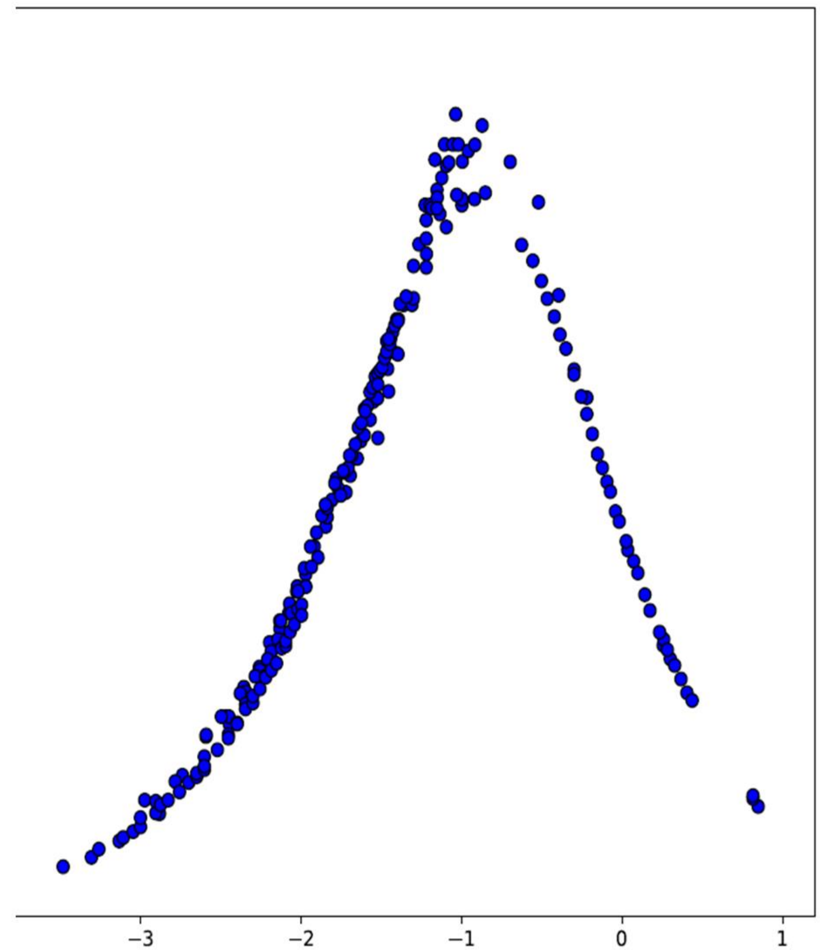


T. Materna, *Université Paris-Saclay, France;* NIMB 505 (2021) 1–16

Data review, Machine Learning and DBSCAN



Impact energy (keV/amu)



Impact energy (MeV/amu)

Conclusions

- IAEA stopping database, main compilation of experimental data, updated 2 or 3 times a year
- Experimental data, still needed
- Reliable values, simulations, online codes, different efforts
- SRIM is a powerful tool, works well in lot of cases, not all. Different codes needs update. ML results, alternative solution
- Theoretical efforts, challenge, different models, high energy stopping is well known, but the maximum and low energy regions not so well, Bragg peak included. Many efforts in progress

Acknowledgments

Technical and financial support from

- National Council of Scientific Research of Argentina,
- University of Buenos Aires
- International Atomic Energy Agency.

Buenos Aires

Thank you!

University of Buenos Aires,
Faculty of Sciences