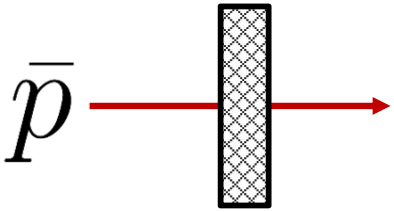
Molecular dynamics simulations of antiproton transmission through energy degrading foils



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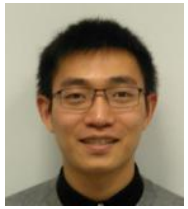

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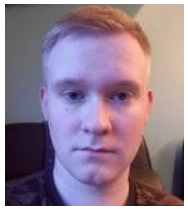
Fusion reactor mat'ls



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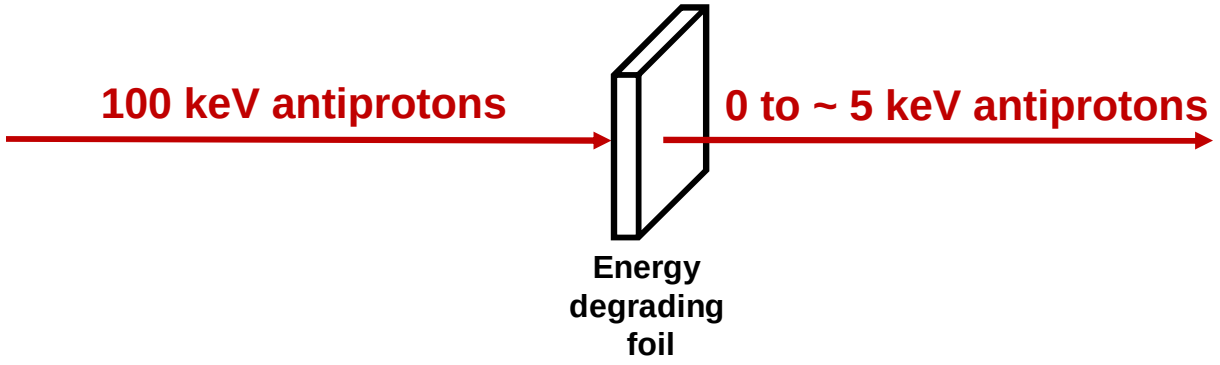
Motivation: how to calculate the slowing down of antiprotons from ELENA in energy degrading foils?

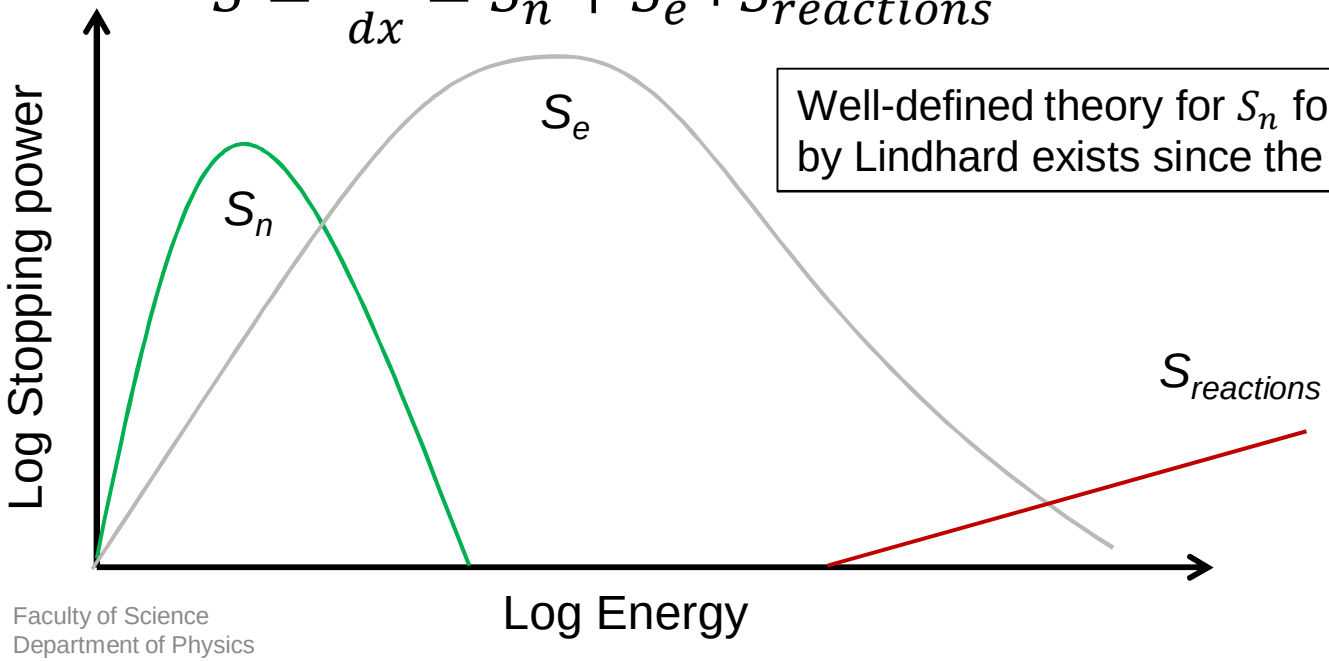


- Key question for improving antiproton yields for $\bar{H}$ production: how to maximize fraction of 0 – 5 keV antiprotons coming through foil?
  - Foil thickness, material?
- To be able to calculate this, we need to be able to calculate **the slowing down** of antiprotons in materials

Basics of ion/anti-ion slowing down

- The slowing down of energetic ions in materials is determined by the **stopping power**
  - Sometimes also called the “linear energy transfer” LET
- Stopping power S is divided into nuclear and electronic components and nuclear reaction parts

$$S = \frac{dE}{dx} = S_n + S_e + S_{reactions}$$



Nuclear stopping power of antiprotons?

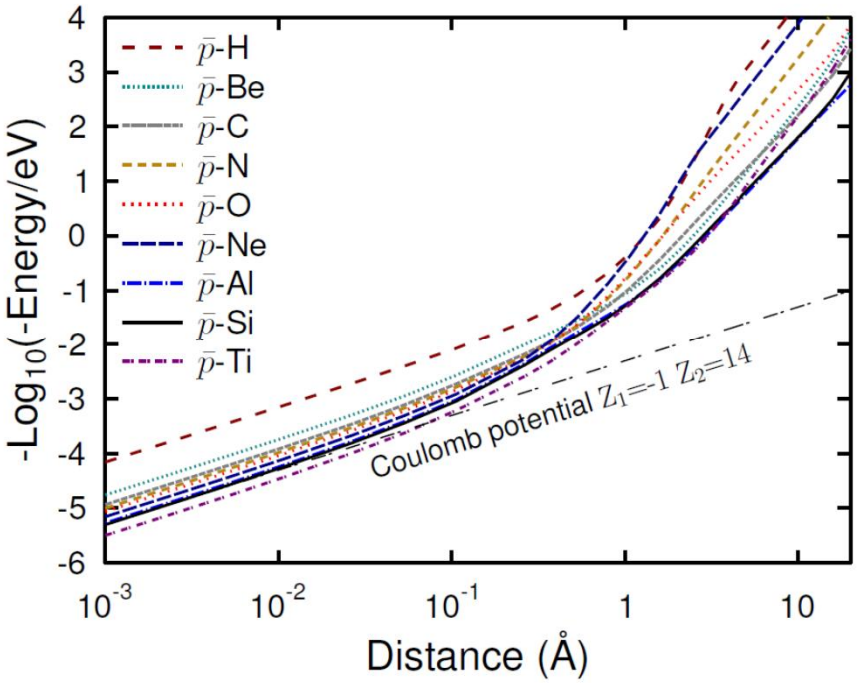
- The electronic stopping power S_e of antiprotons is known from experiments and theory in several materials
- Since we are now interested in energies < 5 keV, also the nuclear stopping power S_n may be of interest

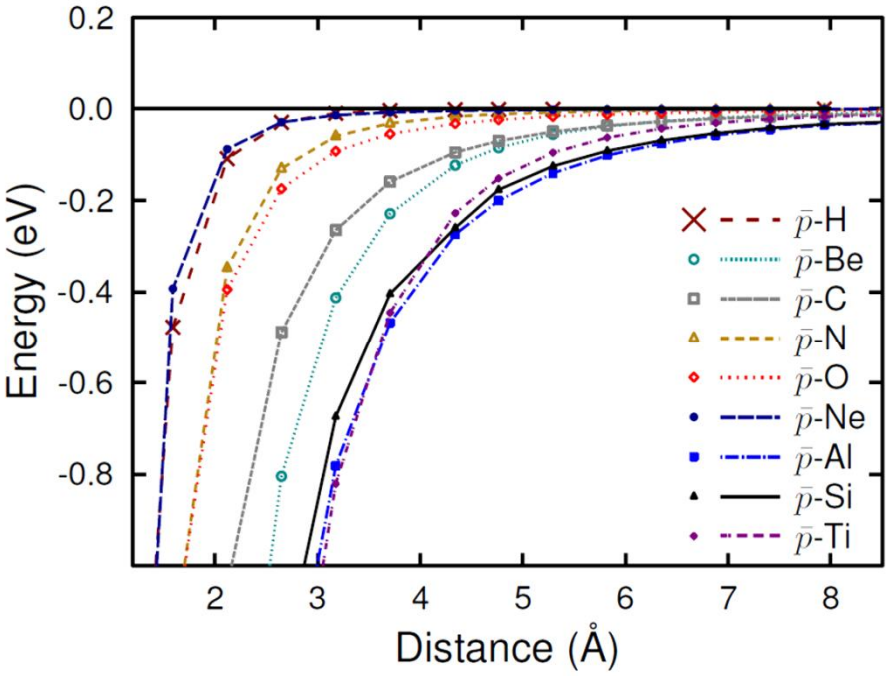
However, turned out nobody ever determined the nuclear stopping power of antiprotons!

- Good enough motivation for doing it now
  - *Hence we basically repeated last 60 years of nuclear stopping theory for antiprotons*

Determining nuclear stopping power of antiprotons, 1.

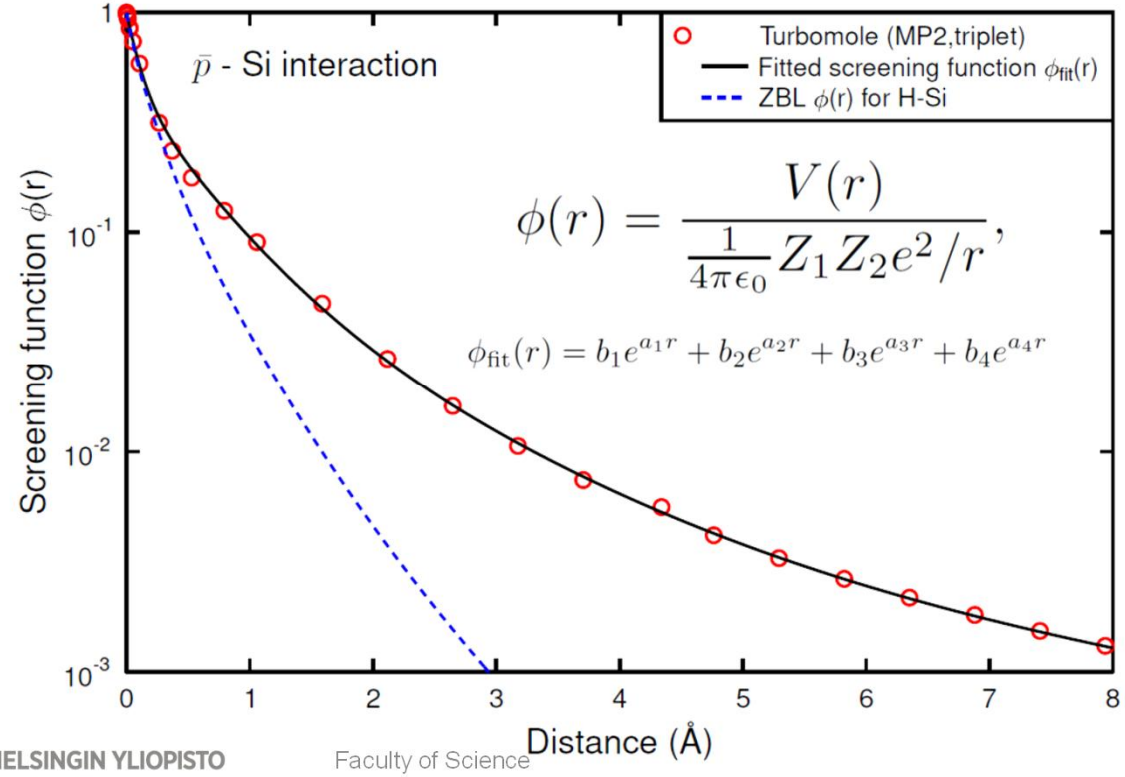
- Step 1: determine interatomic interaction between antiprotons and atoms
  - Quantum chemistry (Hartree-Fock/MP2) with Turbomole code to get total energy of antiproton – atom systems as function of distance
  - DFT also tested, but gave suspicious results





Determining nuclear stopping power of antiprotons, 2.

- Step 2: To enable practical calculations at any interatomic distance, fit screened Coulomb potential to the data
  - Done for 9 elements: H, Be, C, N, O, Ne, Al, Si, Ti



El.	X	X_1	X_2	X_3	X_4
H	b	10.688	0.000319357	0.00597013	$(1-b_1-b_2-$
	a	-2.60175	-0.231507	-0.689763	-2.75173
Be	b	0.00466484	0.525641	0.0277569	$(1-b_1-b_2-$
	a	-0.217729	-1.11801	-0.48179	-7.7278
C	b	0.0380302	0.318996	0.638666	$(1-b_1-b_2-$
	a	-0.612817	-11.2902	-1.84257	-0.193946
N	b	0.0181678	0.765059	0.216198	$(1-b_1-b_2-$
	a	-0.824271	-2.52968	-14.7289	-0.242982
O	b	0.0264826	0.790077	0.182093	$(1-b_1-b_2-$
	a	-0.847469	-2.906	-17.2312	-0.200413
Ne	b	0.000113387	0.00617107	0.116765	$(1-b_1-b_2-$
	a	-0.253027	-0.994693	-24.0586	-3.74468
Al	b	0.00128954	0.0254584	0.276114	$(1-b_1-b_2-$
	a	-0.097406	-0.419499	-1.22892	-7.55095
Si	b	0.00547494	0.360324	0.0913726	$(1-b_1-b_2-$
	a	-0.19811	-1.99426	-0.79267	-9.71705
Ti	b	0.00226208	0.574763	0.135421	$(1-b_1-b_2-$
	a	-0.247931	-3.83816	-0.924926	-18.5785

Determining nuclear stopping power of antiprotons, 3.

- Step 3: Use classical scattering theory of binary collisions to calculate energy loss in binary collisions and by integrating this, get nuclear stopping power

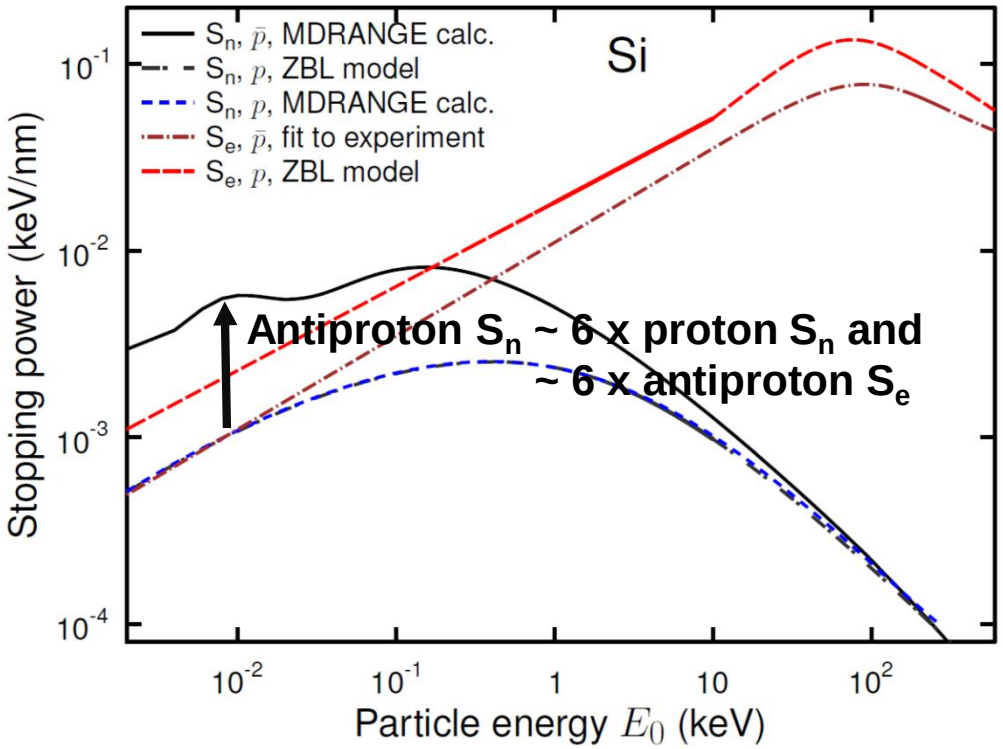
$$S_{\mathrm{n}}(E_0) = N \int_0^\infty T(E_0, b) d\sigma = 2\pi \int_0^\infty T(E_0, b) b db$$

(b is the impact parameter of the binary collision)

- Note that since the potentials are attractive, the trajectories are not necessarily hyperbolic: binary collision approximation cannot be used, needed to use molecular dynamics!

Nuclear stopping power of antiprotons: results

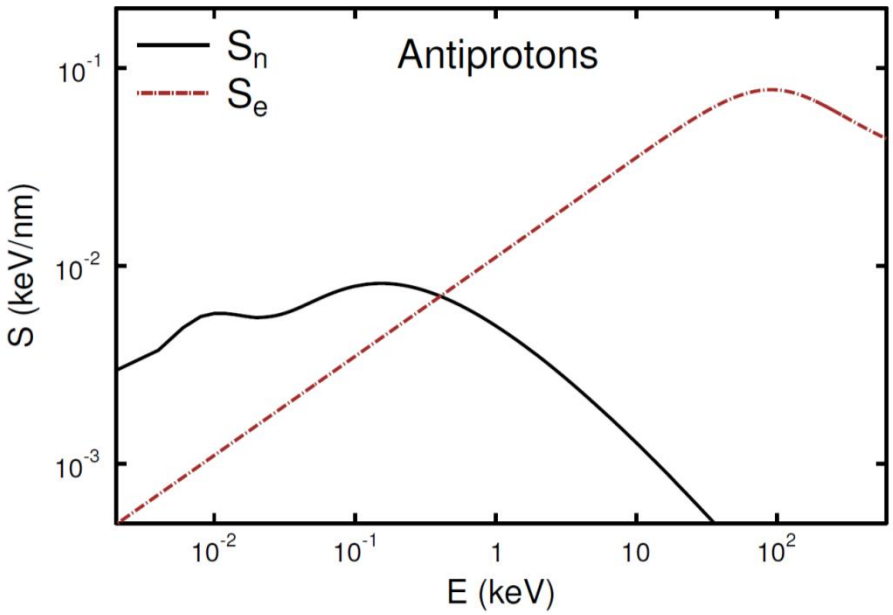
- Results show that:
  - 1. The nuclear stopping power S_n of antiprotons can be stronger than their electronic stopping power (contrary to protons)
  - 2. It is much stronger than that of protons

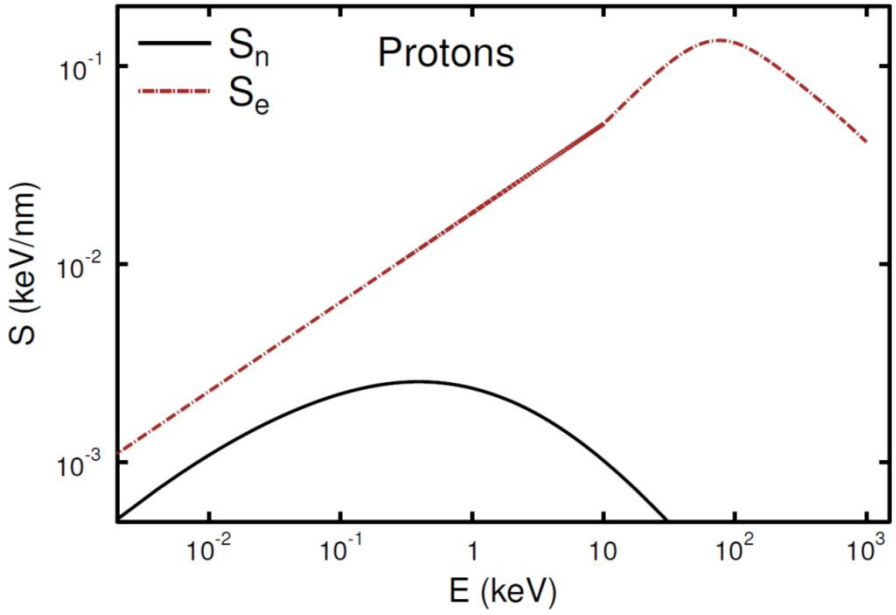


[K. Nordlund, D. Sundholm, P. Pyykkö, D. Martinez Zambrano, and F. Djurabekova, Phys. Rev. A **96**, 042717 (2017)]

Nuclear stopping power of antiprotons: results

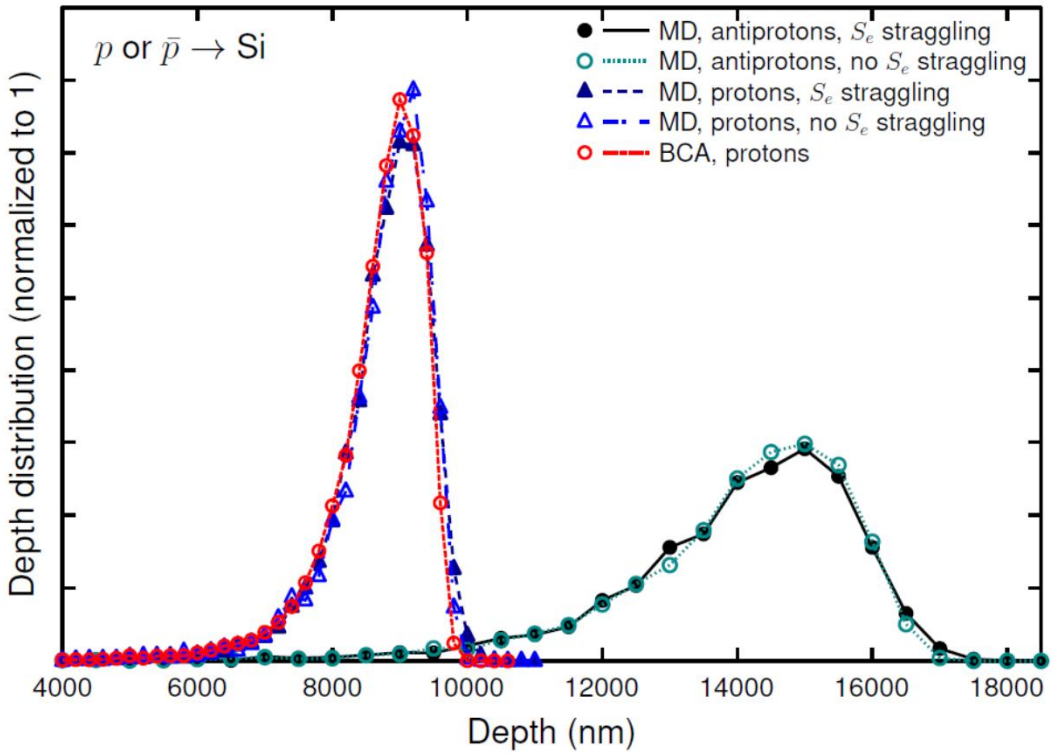
Ø Summary comparison of antiprotons and protons





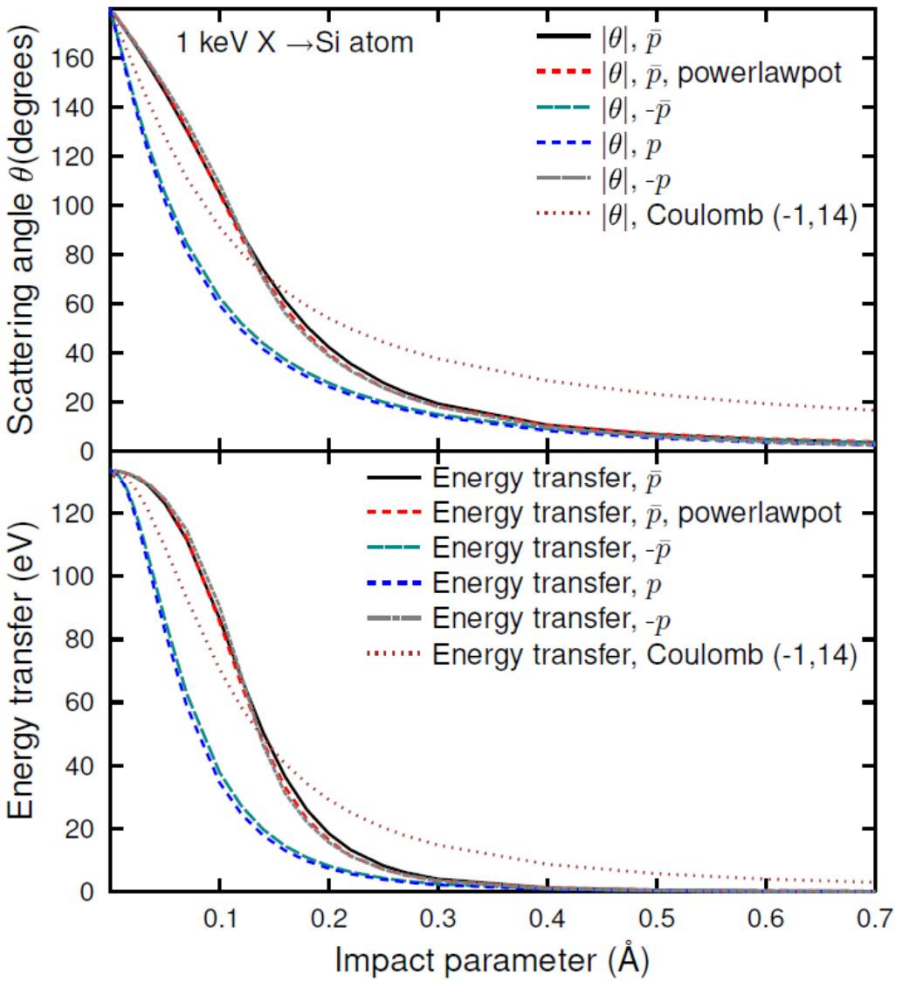
Comparison of proton and antiprotons range profiles

- Range profile simulations for protons give very different results, as expected



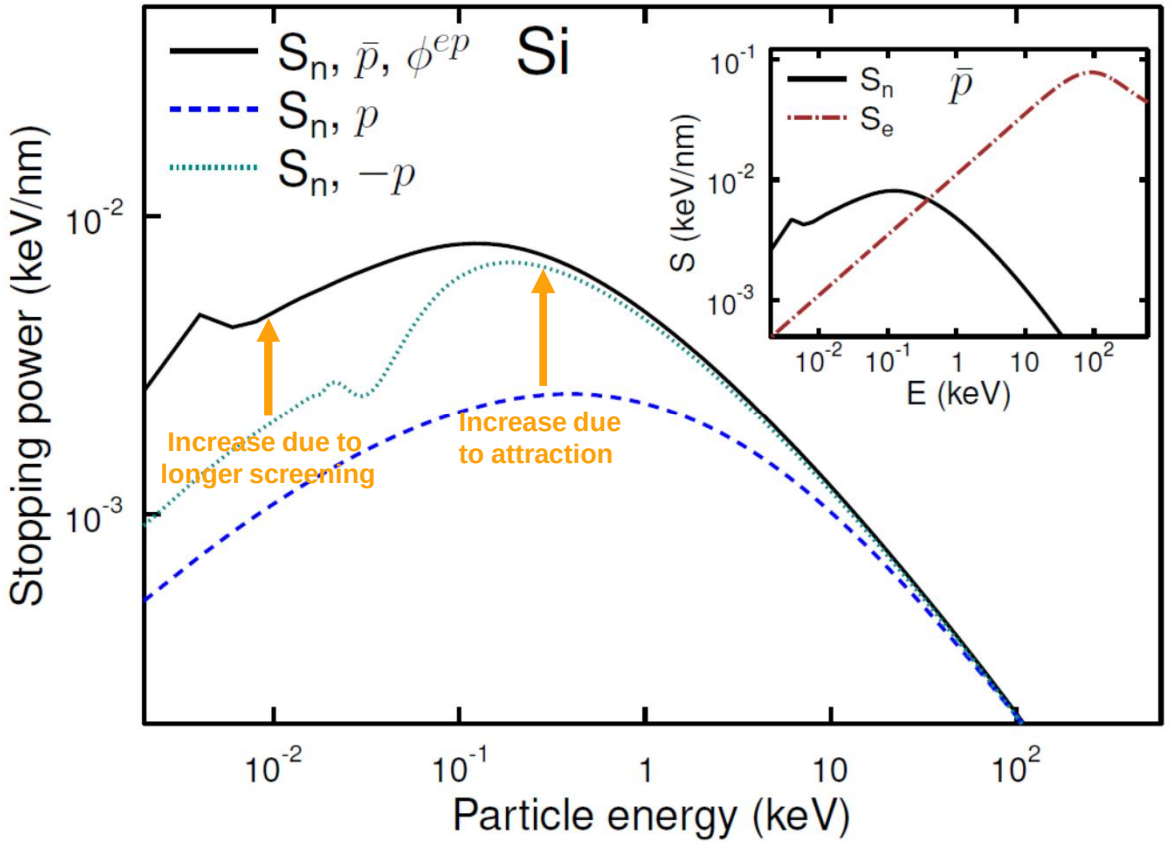
Reason to stronger stopping

- To understand the origin of the stronger stopping, we analyzed the scattering angle and energy transfer as a function of the impact parameter for 1 keV
- Clearly larger scattering and energy transfer for antiprotons $\bar{p}$ than protons p
  - Note that a hypothetical "negative proton $-p$" has similar behavior as the antiproton $\bar{p}$



Reason to stronger stopping

- Comparison of antiprotons, protons and hypothetical "negative proton" shows that both attraction and longer screening length leads to increased nuclear stopping power

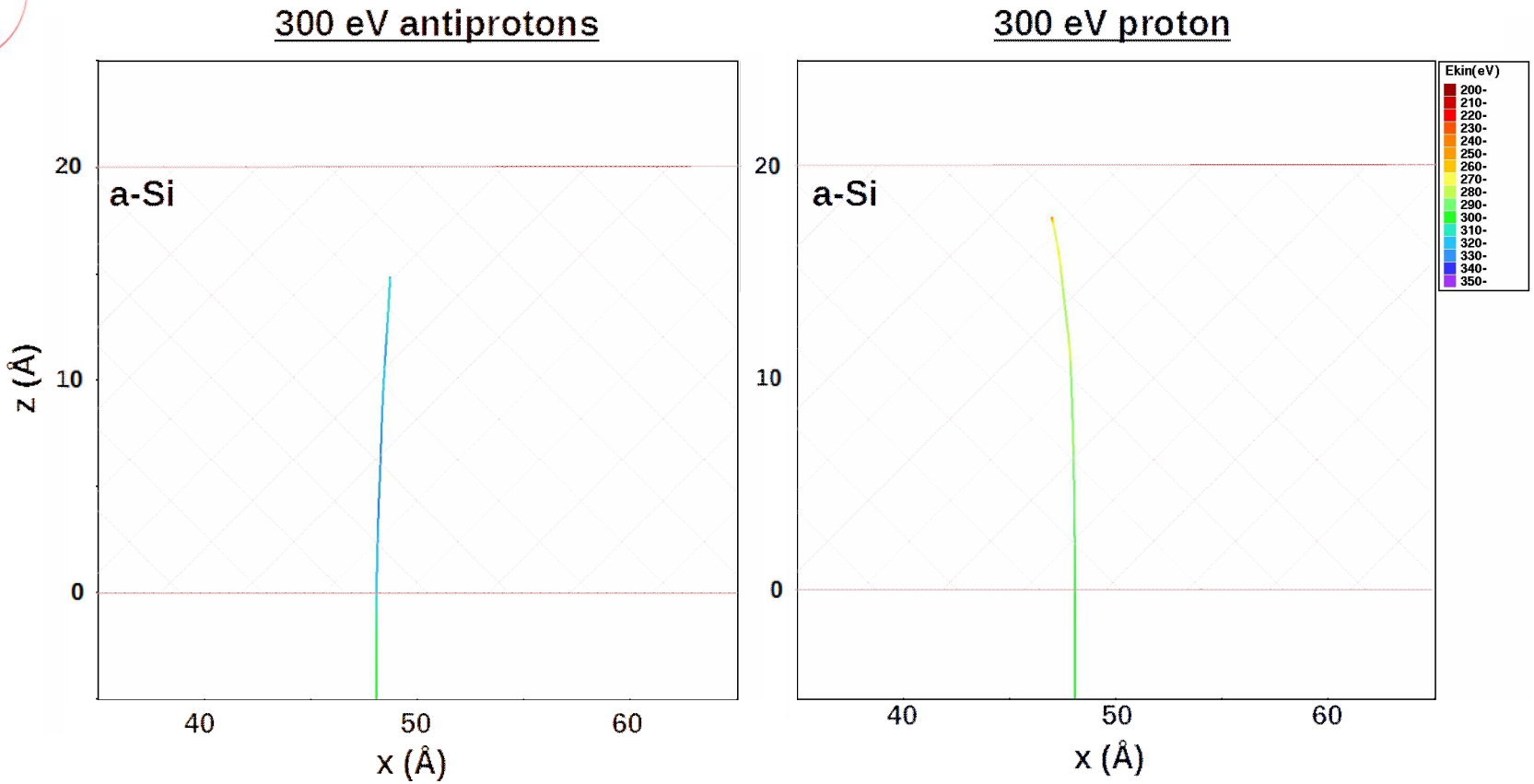


Molecular dynamics of antiproton transmission through foils

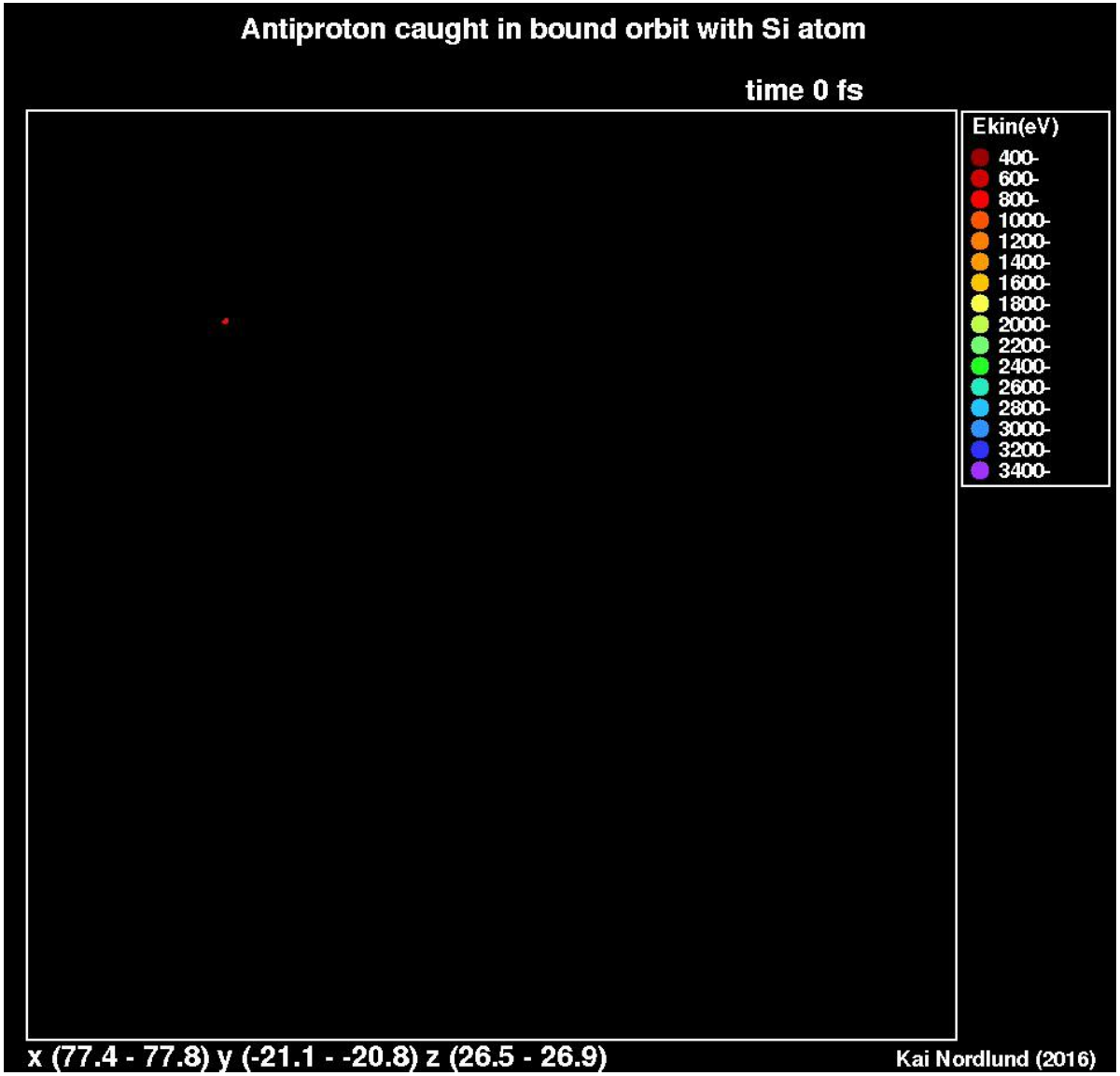
- However, to calculate the transmission through foils, one needs actual trajectory simulations, as the antiprotons do not move in straight paths
- Hence we did MDRANGE (MD in recoil interaction approximation) simulations of antiproton movement in the foils
  - In some cases, the antiprotons were captured in the purely attractive potential: observed spiral path inwards, or Kepler-like bound orbit
  - Hence cutoff criterion introduced: if antiproton came within 3 nm of nucleus, a nuclear reaction was assumed to occur and the simulation was stopped

Molecular dynamics of antiproton transmission through foils

Ø Animation: transmission of 300 eV $\bar{p}$ through 2 nm Si foil

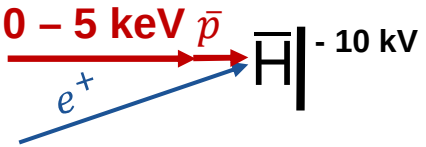


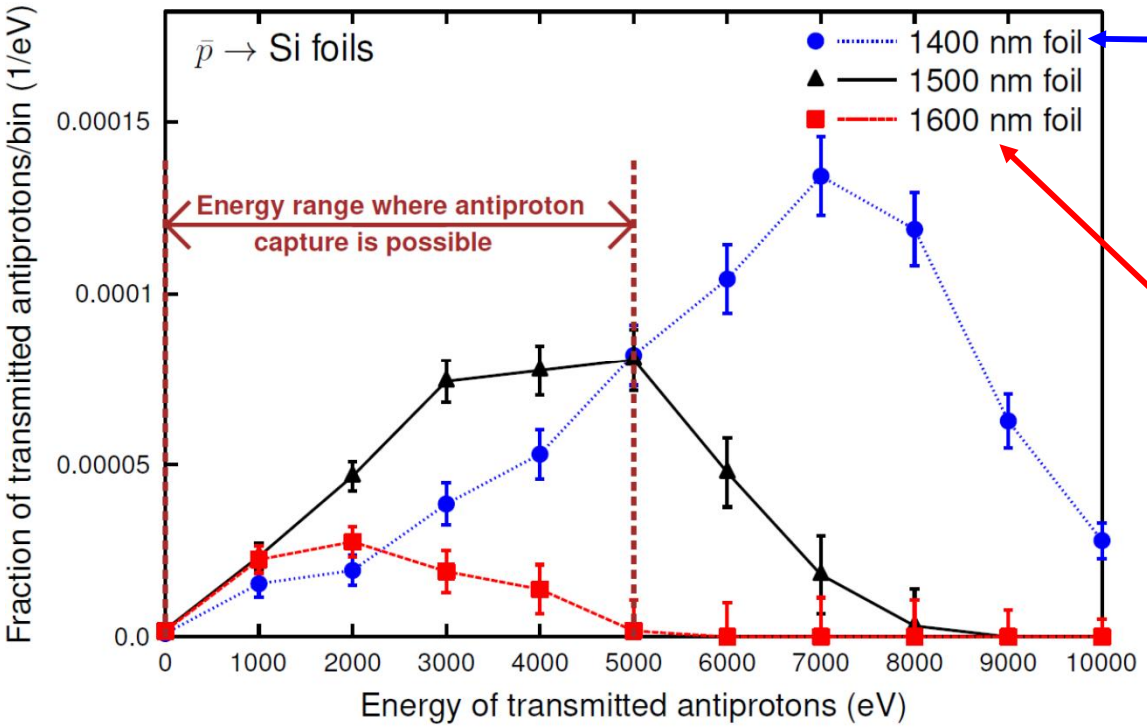
Antiproton in Kepler orbit: animation



Simulations of practical importance: optimization of foil thickness, 1.

- The aim for the ATRAP experiment is to find foil materials and thicknesses that optimize for incoming 100 keV $\bar{p}$ the transmitted fraction of 0 – 5 keV ones



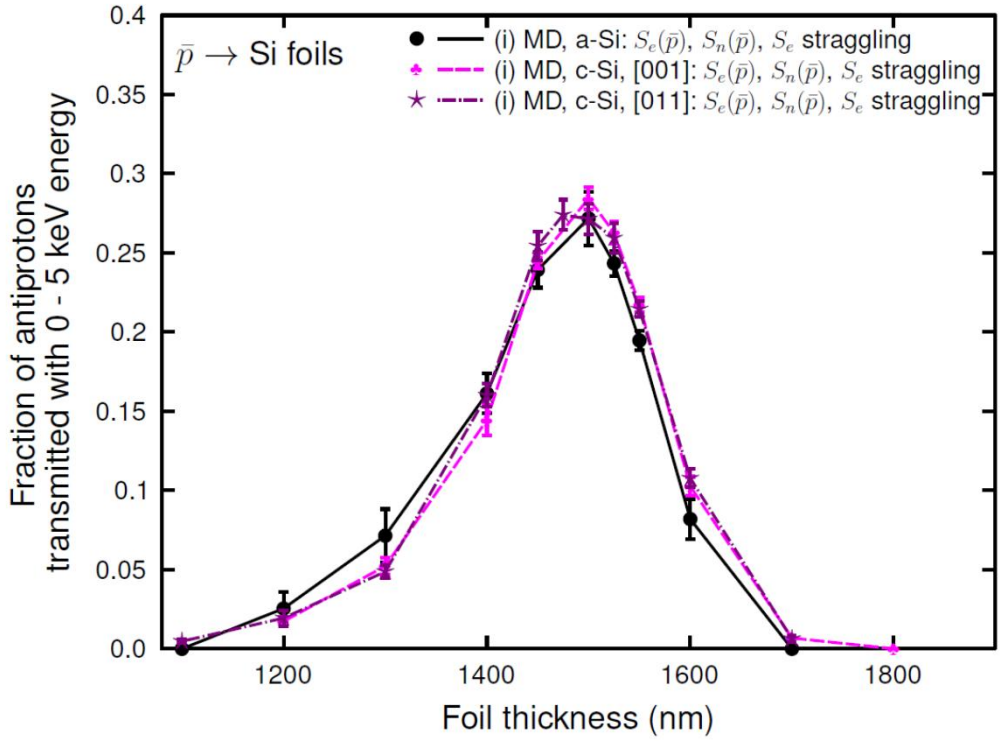


Too thin foil: energy of transmitted particles too high

Too thick foil: little or no transmission

Simulations of practical importance: optimization of foil thickness, 2.

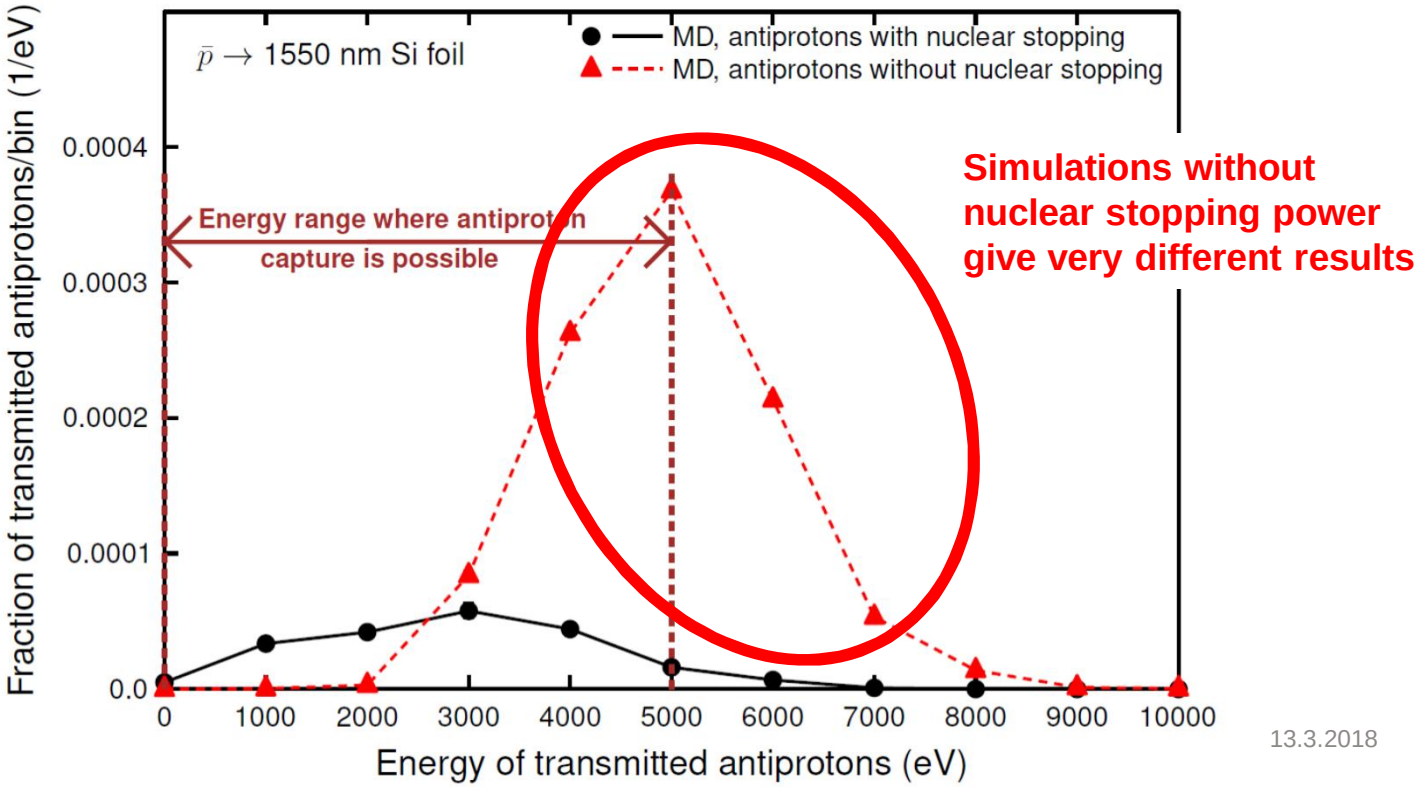
- By integrating the fraction of antiprotons transmitted through the foil with energy between 0 and 5 keV for various thicknesses, we could find the optimal thickness
- Predicted optimal thickness for a-Si and c-Si foils: 1500 nm



[**K. Nordlund**, D. Sundholm, P. Pyykkö, D. Martinez Zambrano, and F. Djurabekova, Phys. Rev. A **96**, 042717 (2017)]

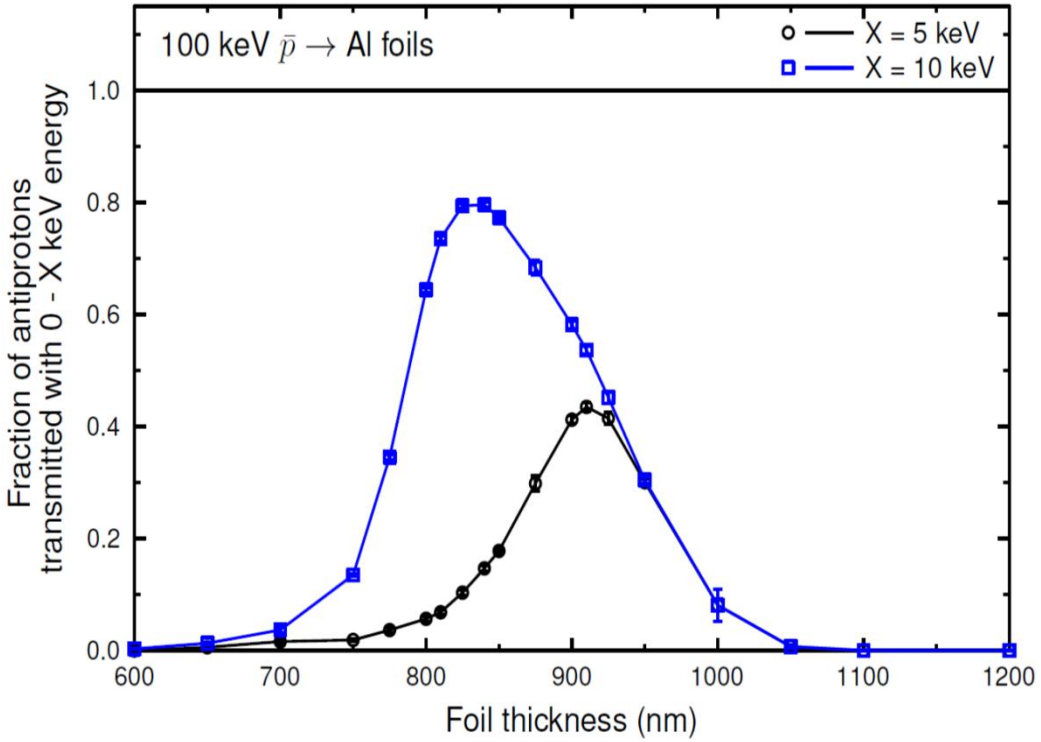
Simulations of practical importance: does the nuclear stopping actually matter?

- We also tested whether doing all the trouble of including the nuclear stopping actually matters
- Answer: yes it does!



Optimization of Al

- We also did a similar optimization run for Al, as Al foils are likely easier to use than Si.
- Result: optimal thickness 900 nm (5 keV max)



[K. Nordlund, Results in Physics 8 (2018) 683]

Conclusions

- Using modern quantum chemistry, we determined interatomic potentials between antiprotons and 9 different elements
- These can be used for a) determining the nuclear stopping power and b) molecular dynamics simulations of antiproton movement in materials
- Results show that the nuclear stopping power of antiprotons is stronger than their electronic stopping at low energies, and also always stronger than that of protons
- Enables optimization of energy degrading foil thicknesses w.r.t. the transmitted fraction of antiprotons

[K. Nordlund, D. Sundholm, P. Pyykkö, D. Martinez Zambrano, and F. Djurabekova, Phys. Rev. A **96**, 042717 (2017)]

Backup slides

Atomic polarizability

- The TurboMole calculations allowed calculating atomic polarizabilities comparable to experiments

TABLE I. Comparison of the atomic polarizabilities, α, (in a.u.) from the present Eq. (1) using MP2 data to literature values. 'PW' = present work.

Atom	Polarizability, α	
	PW	Lit.
Be	40.90	37.76^{a}
N	5.34	7.63^{b}
Ne	2.44	$2.66110(1)^{c}$

^{a} Ref. [41], ^{b} Ref. [42] (exp), ^{c} Ref. [43] (exp).

Atomic polarizability

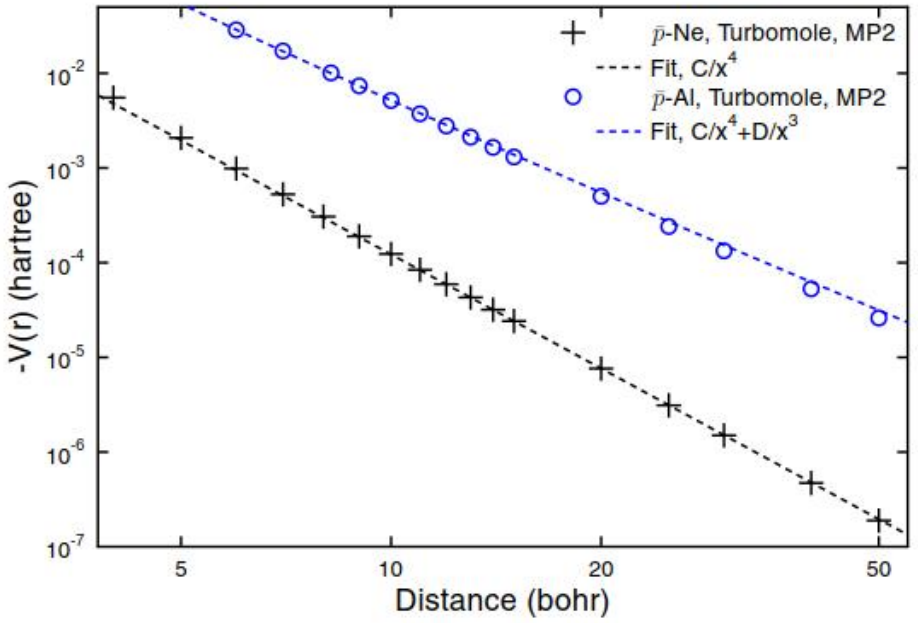


FIG. 4. The calculated MP2 antiproton-neon and antiproton-aluminum potentials (symbols) at large separations and a fit to $V(r) = -C/2r^4$ with $C = 1.222$ hartree for Ne and $V(r) = -C_3/r^3 - C_4/r^4$ with $C_3 = 3.611$ and $C_4 = 15.675$ hartree for Al.

Different screenings

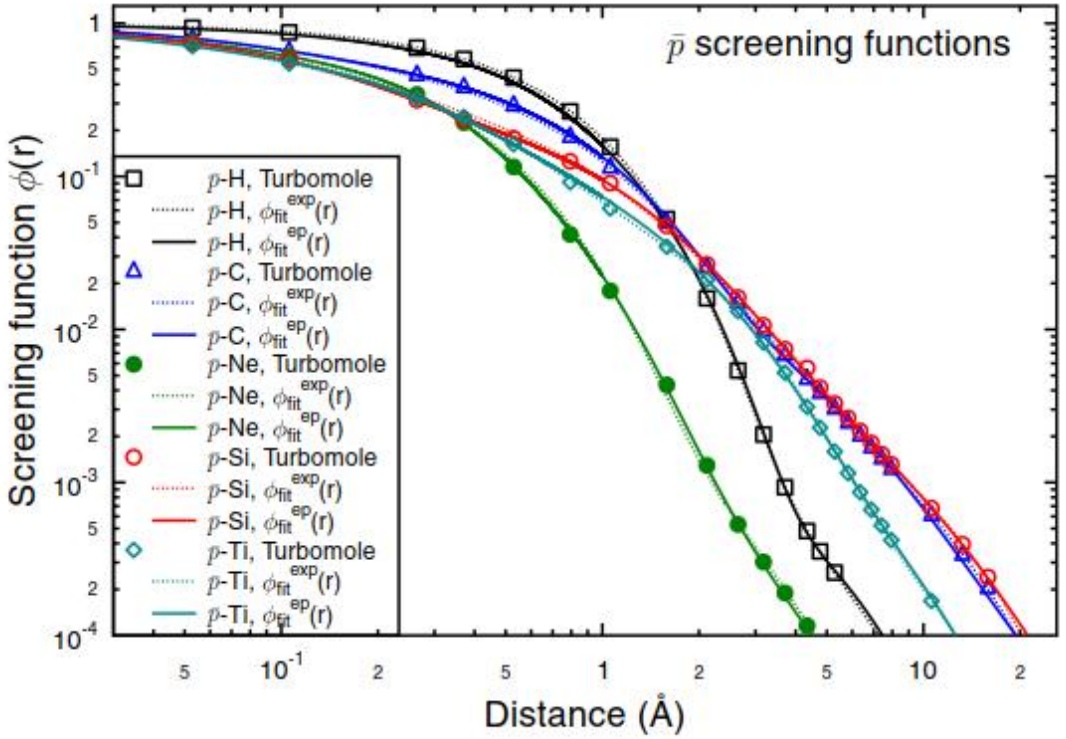
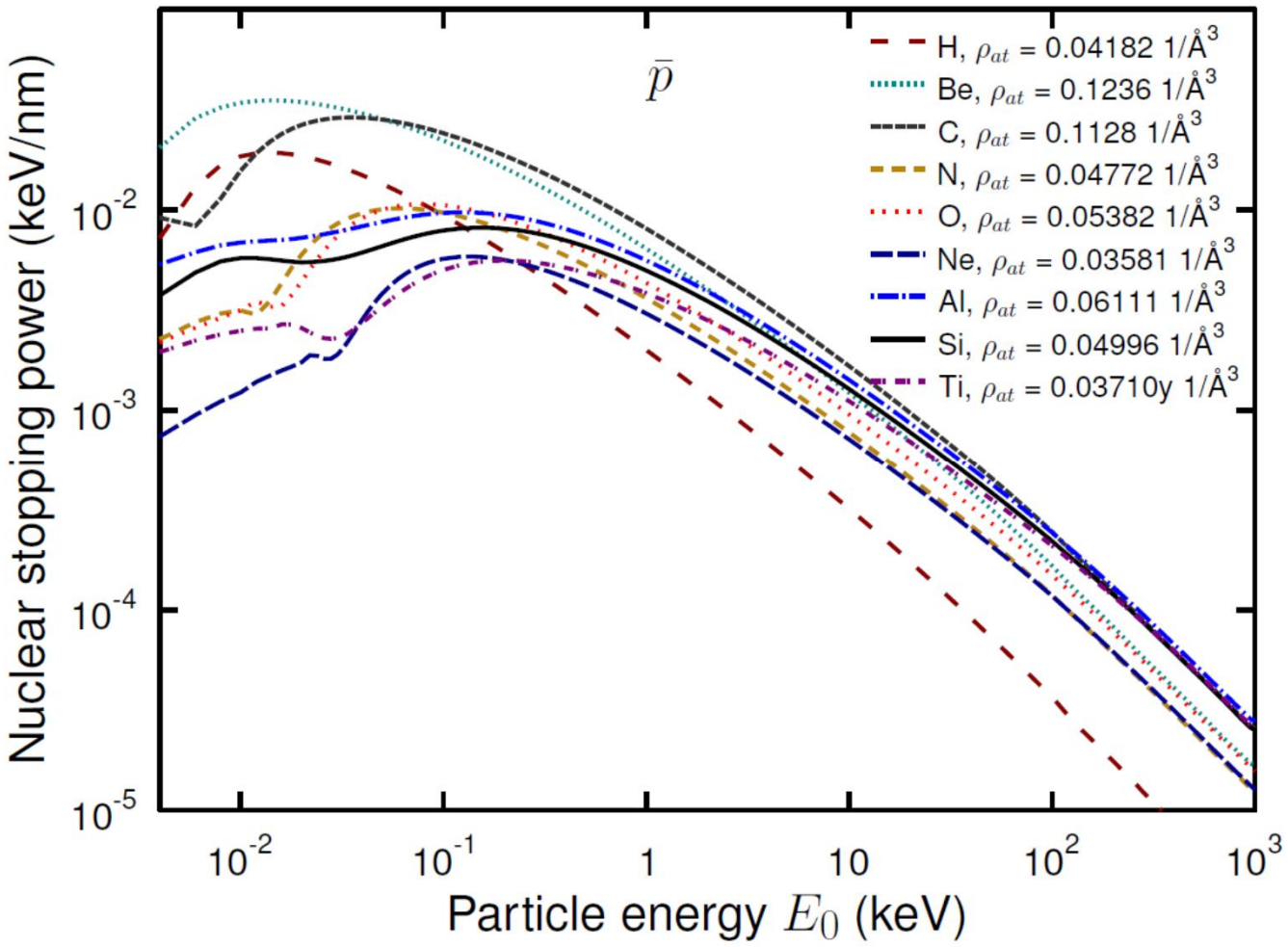
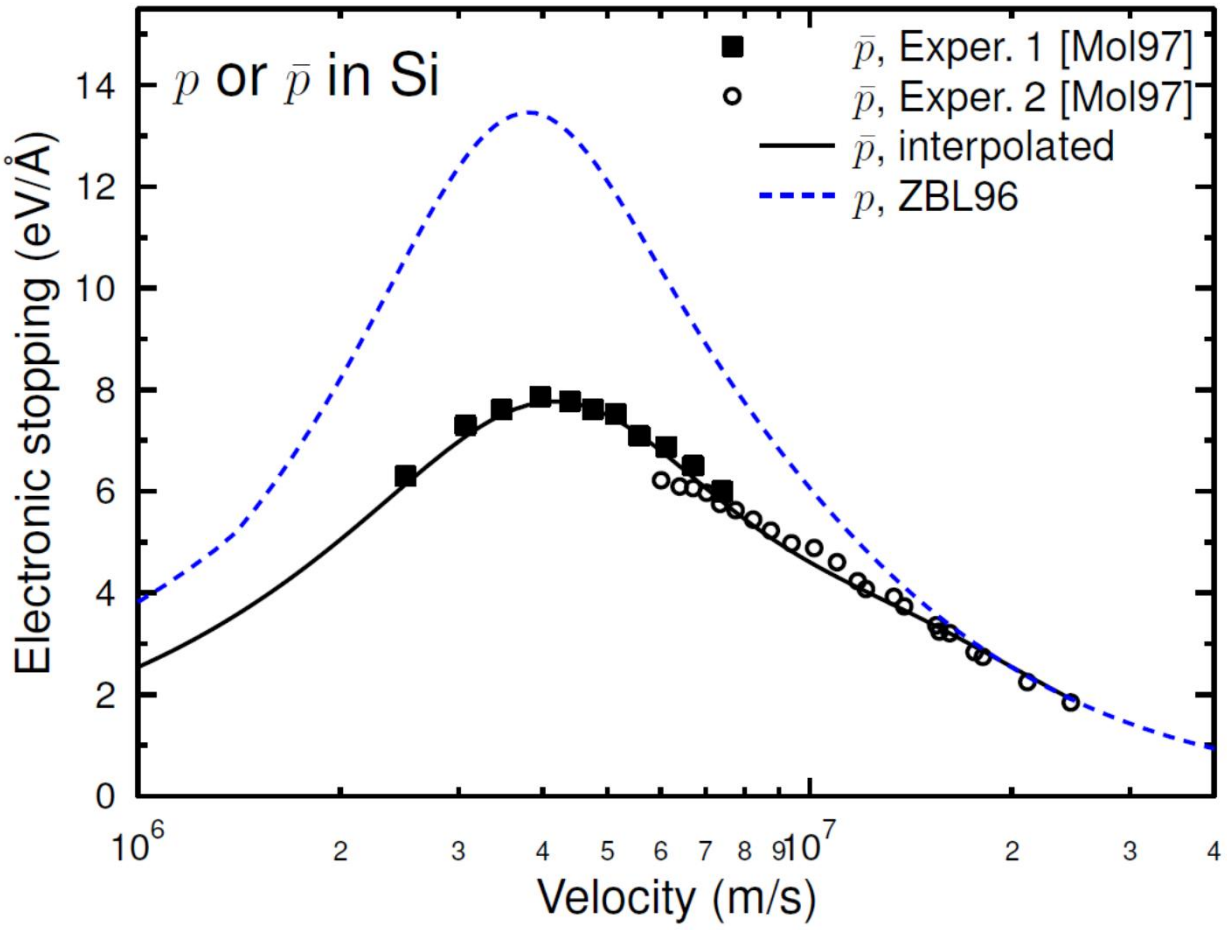


FIG. 5. Comparison of screening function fits obtained with the two different functional forms $\phi_{\rm fit}^{\rm exp}$ and $\phi_{\rm fit}^{\rm ep}$.

All nuclear stopping powers

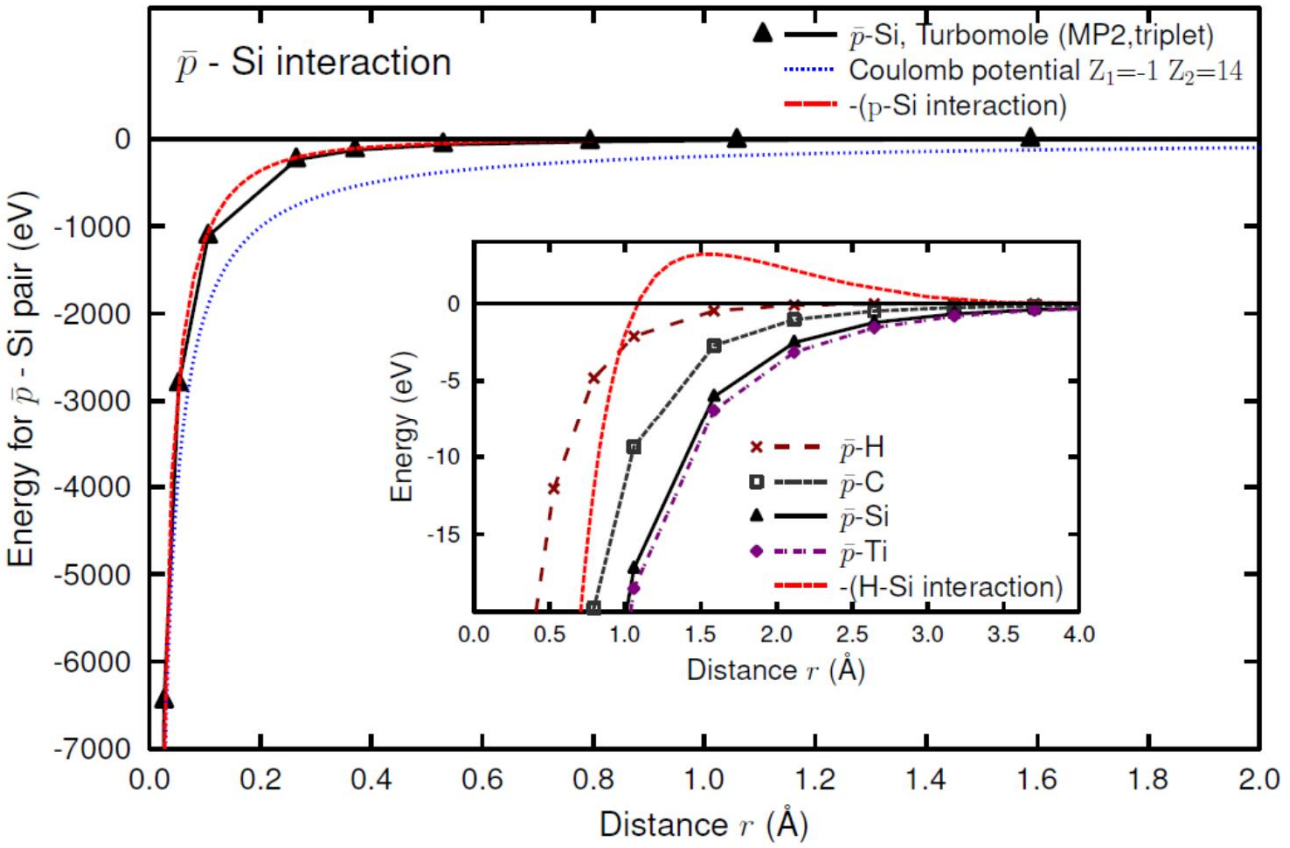


Electronic stopping of antiprotons in Si

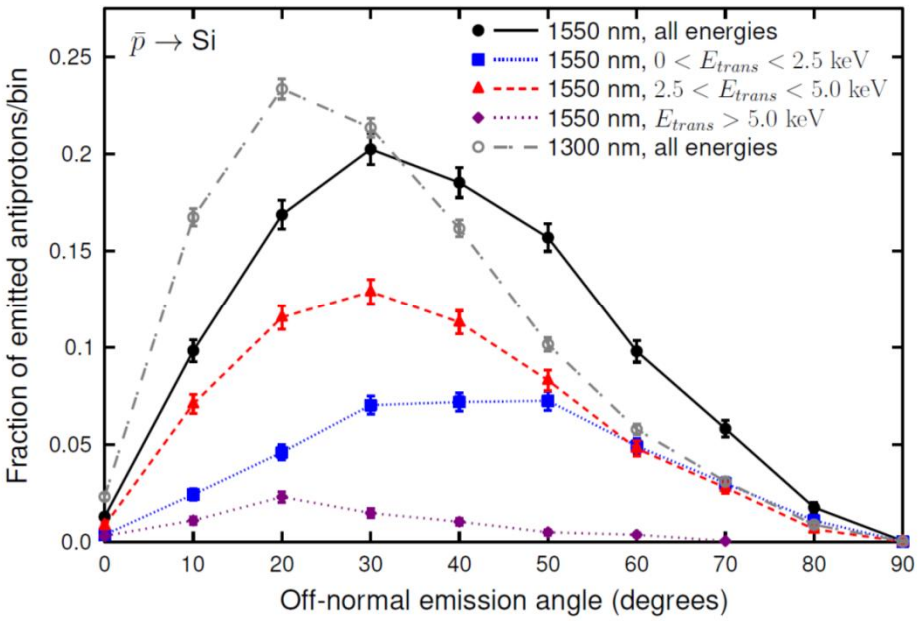


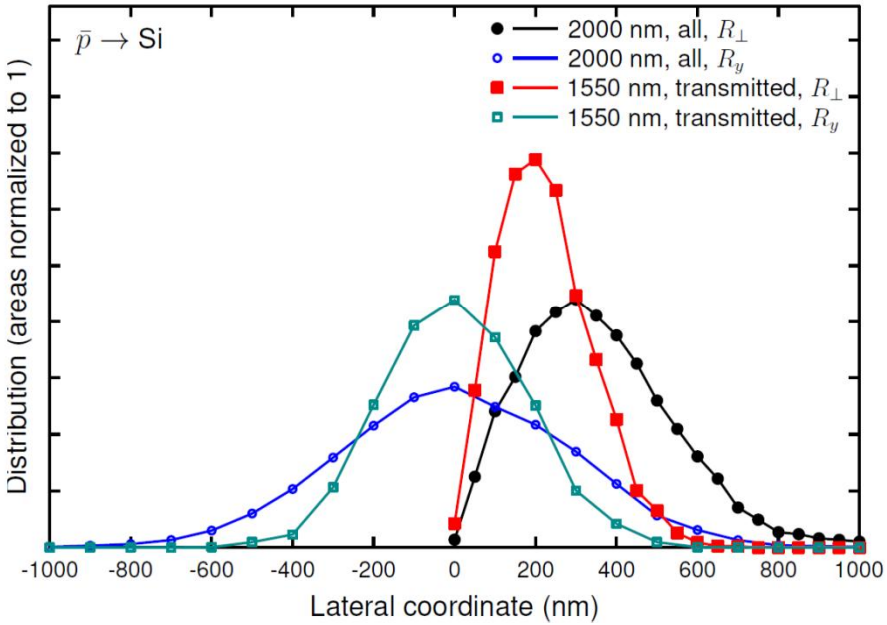
Comparison with p-Si and H-Si

Ø Comparison with p-Si and H-Si

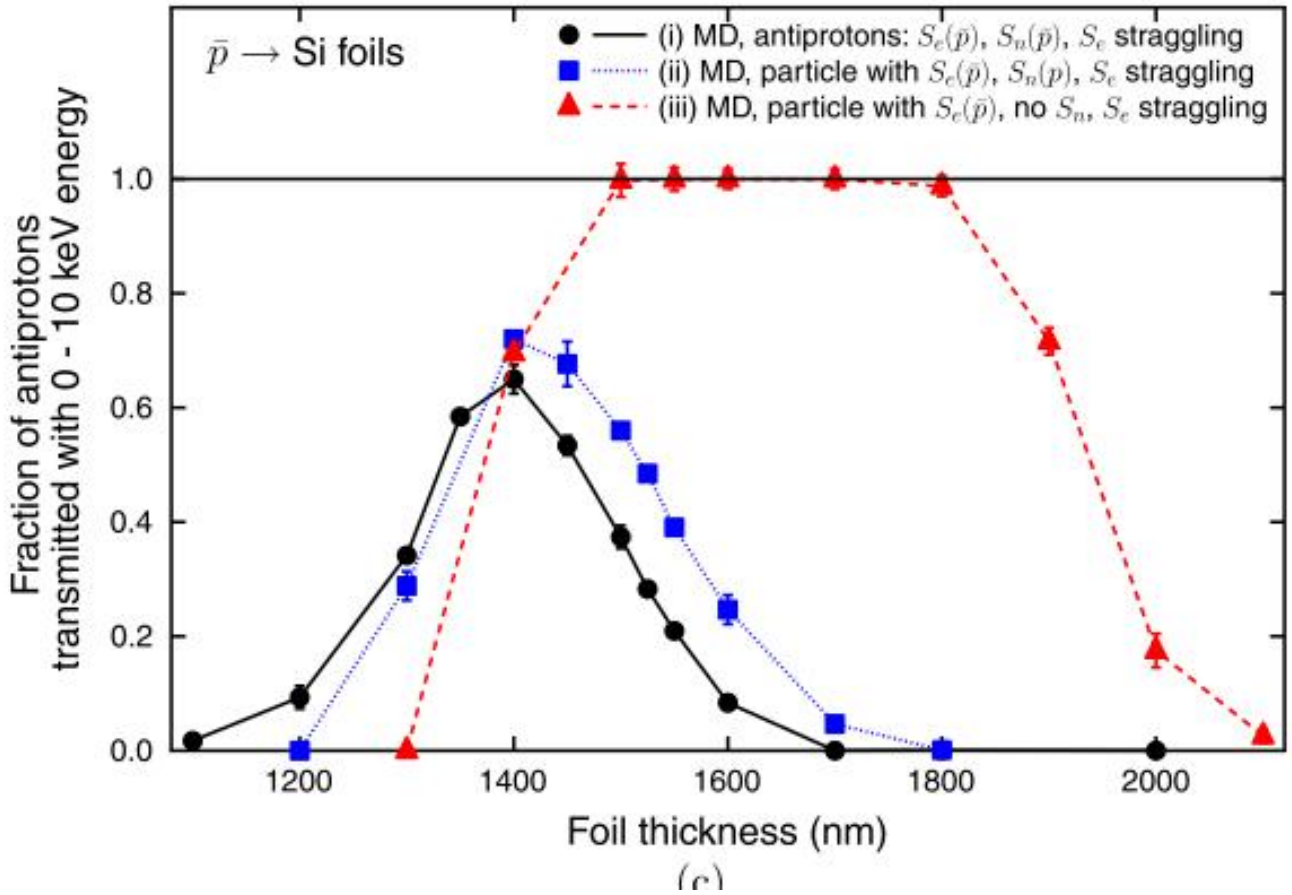


Angular and lateral spread on exit





With 10 keV upper limit



Background: antihydrogen production at CERN