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Electronic stopping in warm dense matter using Ehrenfest dynamics and time-dependent density functional theory

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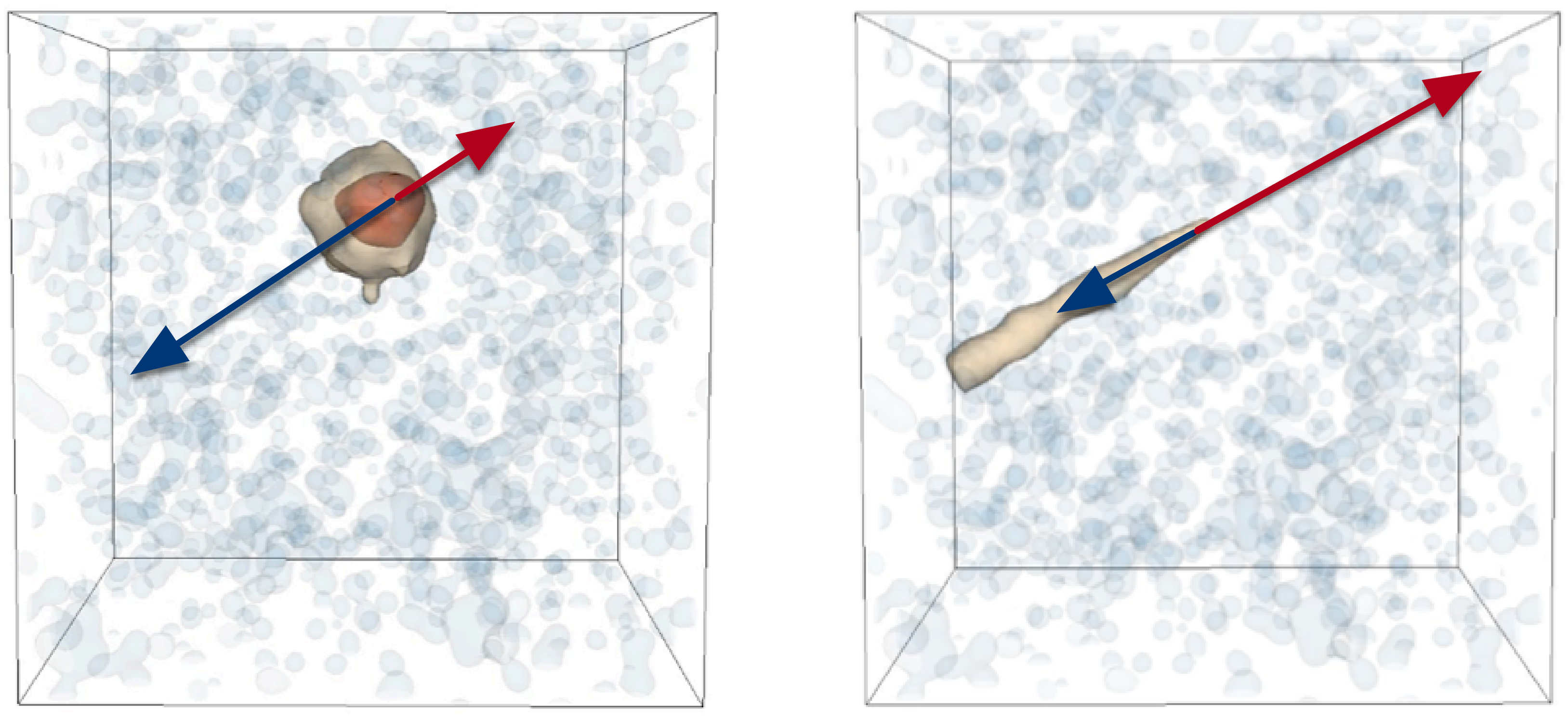
Motivation

Stopping power models are a critical component of hydrodynamic models and responsible for accurately describing **self-heating processes** vital to fusion.

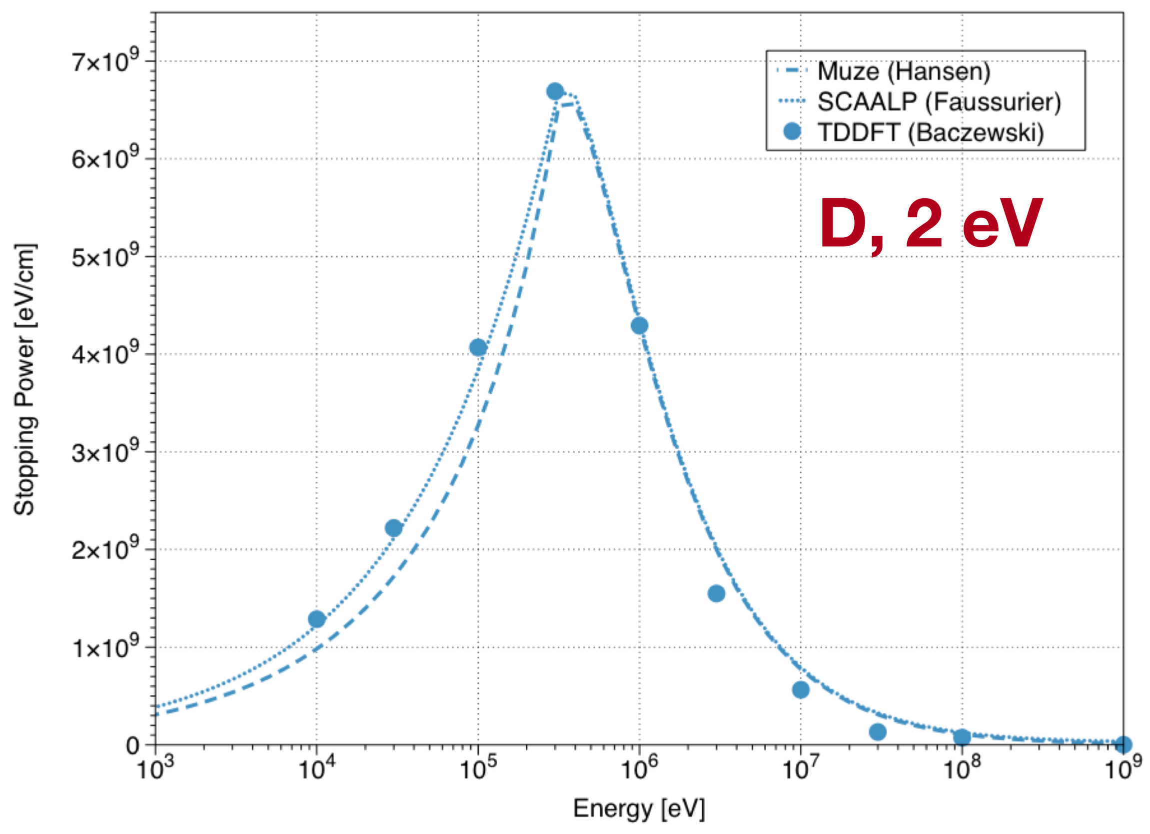
Simple picture: **velocity-dependent resisting force**



+1 charge passing through **deuterium** at **2 eV, 10 g/cm³** at (left) **300 keV** and (right) **30 MeV**

Methods

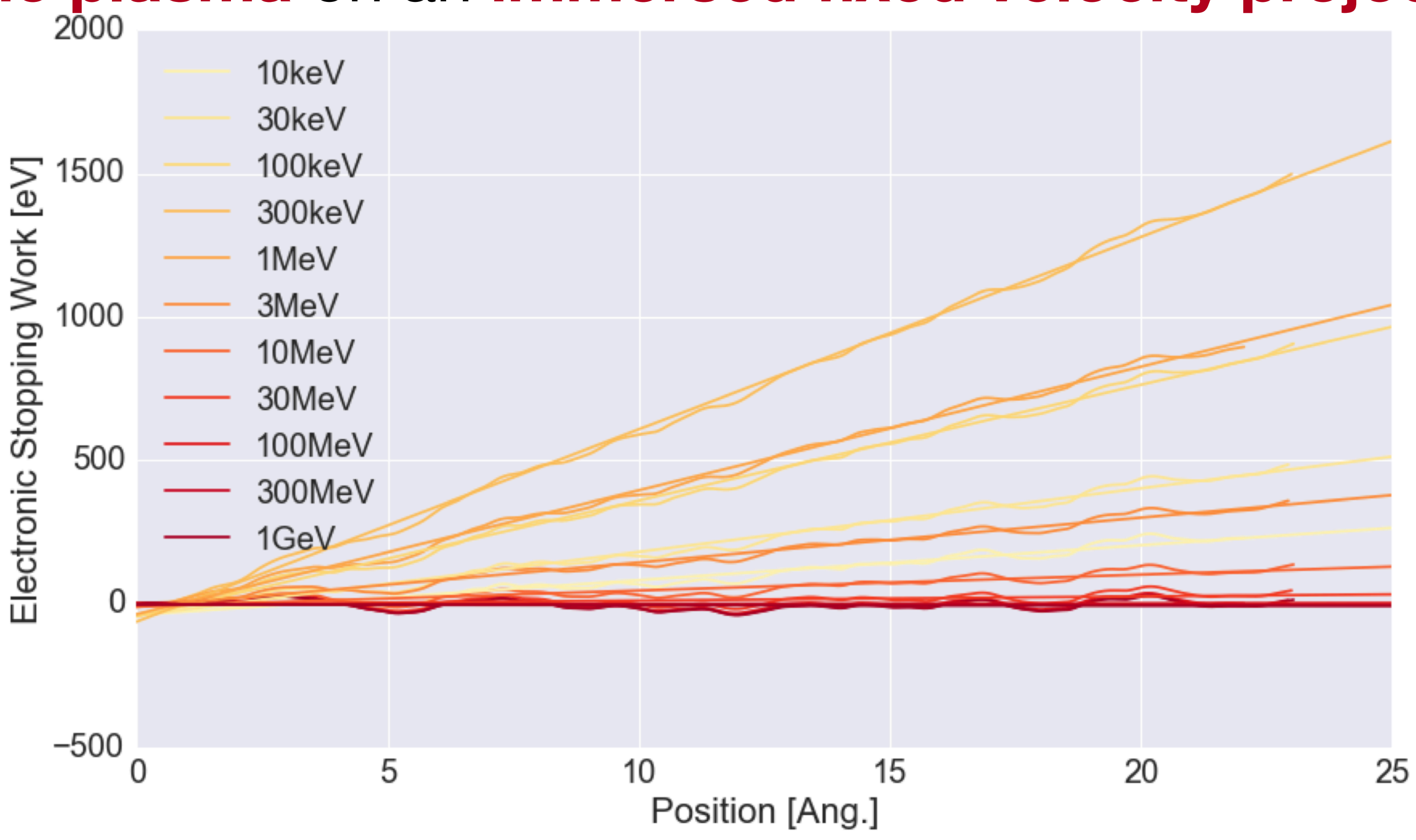
Microscopic models can be separated into **expensive first principles** and **inexpensive semi-empirical models**



Average-atom (AA) models compare quite well to **Ehrenfest-TDDFT** for warm dense deuterium **[1]**

AA ultimately relies on local density-dependent **dielectric response models** and the **most accurate treatment of collisions** remains an open question, especially for **atoms with more complex electronic structure**.

Ehrenfest-TDDFT relates stopping power to **work done by the plasma** on an **immersed fixed velocity projectile**



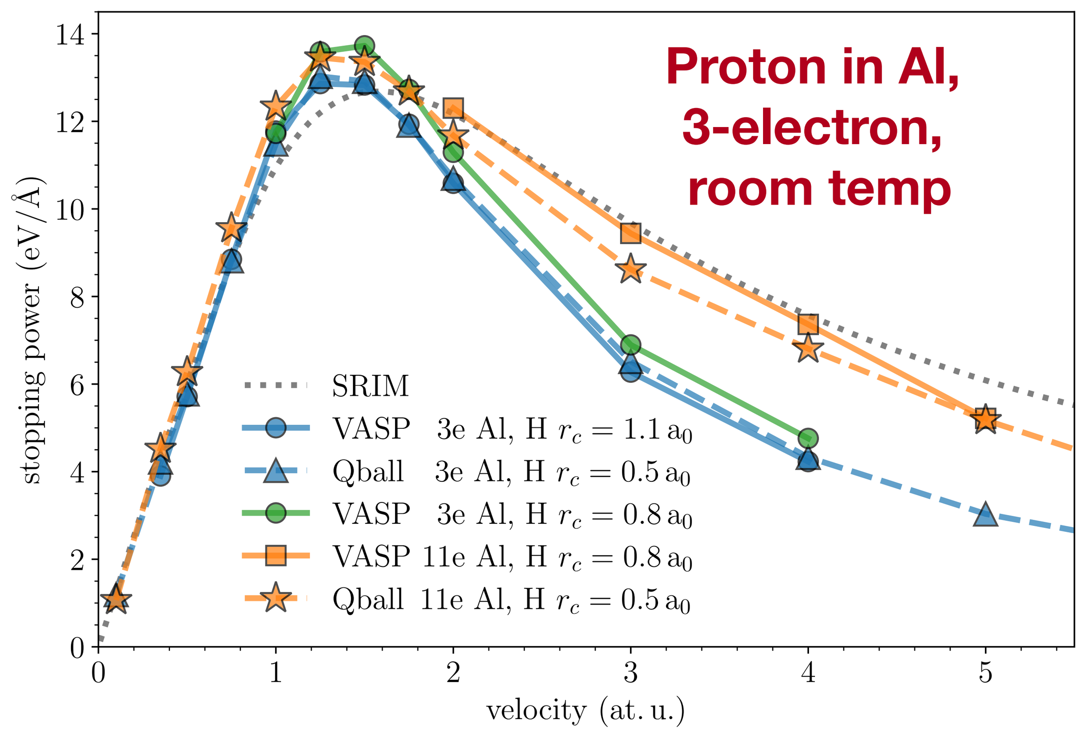
Accuracy depends on

1.) exchange-correlation model **(weak)**,
2.) pseudization scheme **(strong)**,
3.) finite-size effects **(velocity-dependent)**

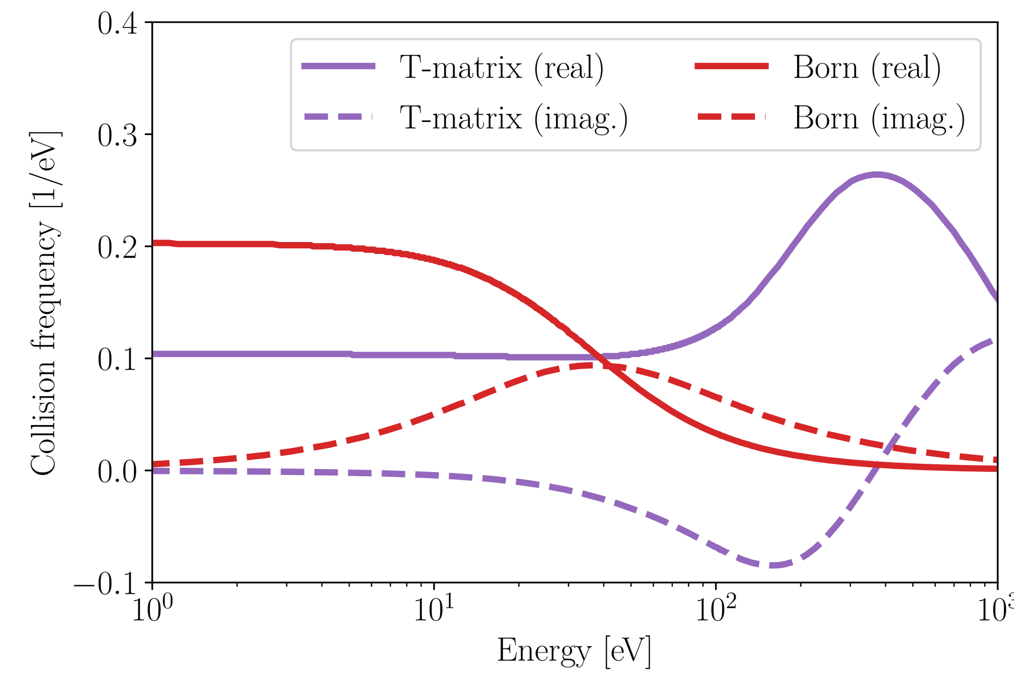
Aluminum results

Our **VASP implementation [2,3]** is based on the highly accurate **projector augmented-wave formalism [4]**

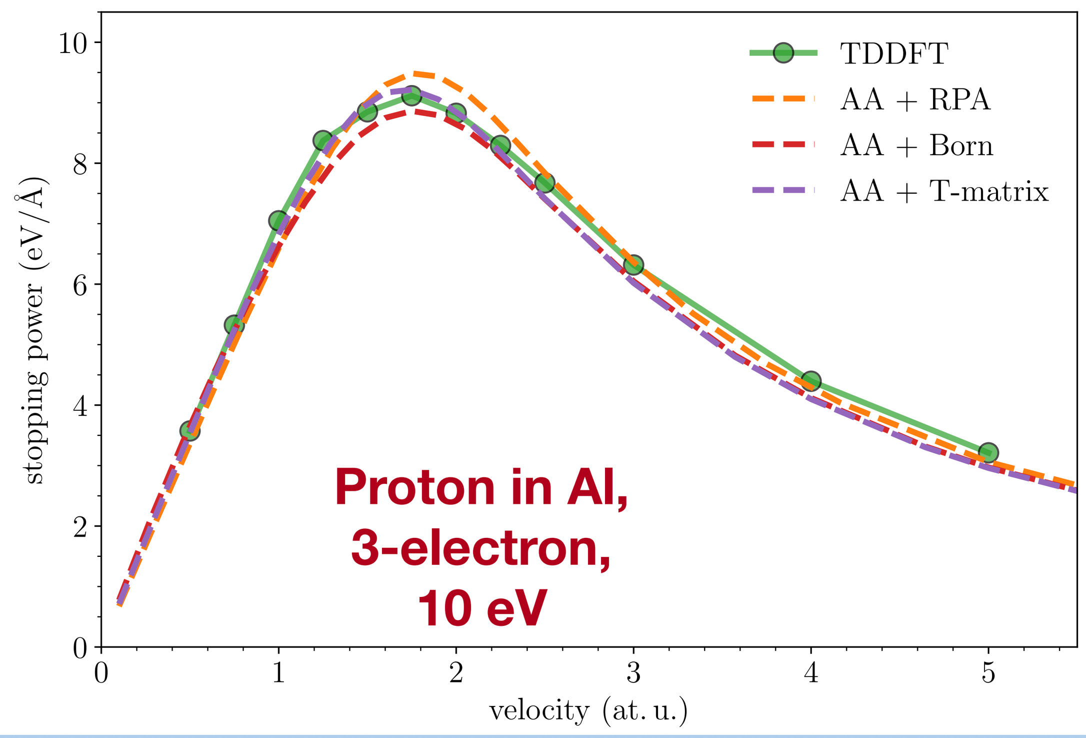
We compare to **Qball**, which makes use of **norm-conserving pseudo potentials [5]**, and **SRIM [6]**.



We next consider **isochorically heated aluminum**, comparing TDDFT to different collisional models in AA

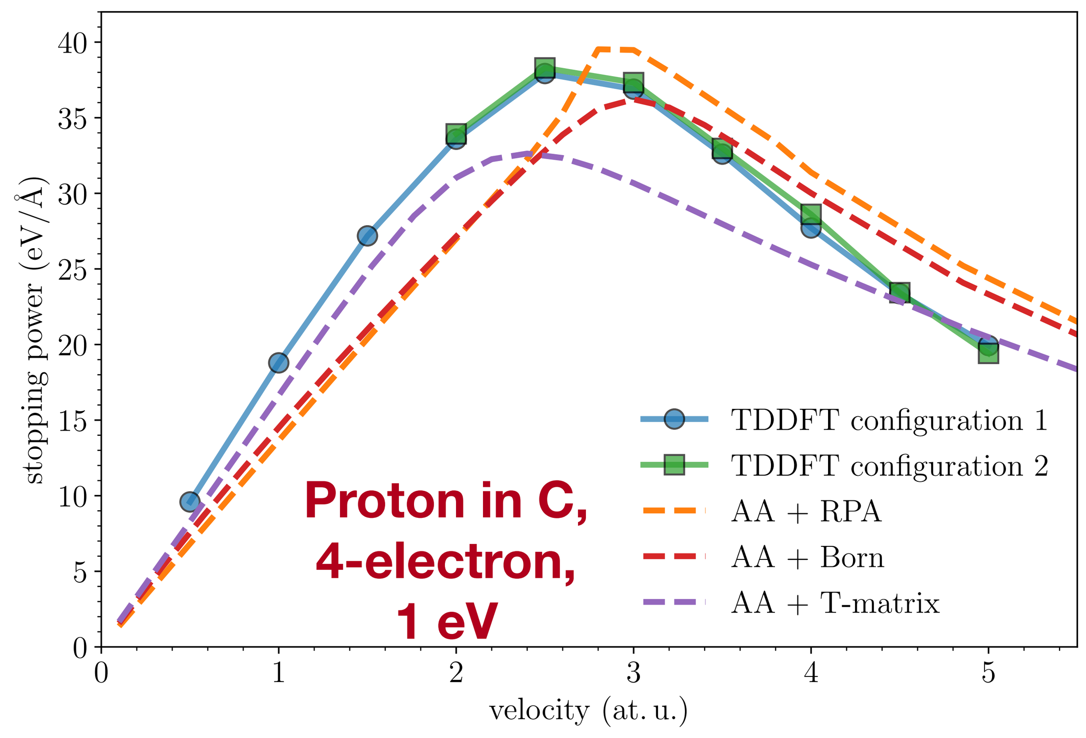


3-electron Al benchmarks **free-electron stopping** in AA.



Carbon results

4-electron carbon is a less ideal free-electron system.



Warm dense conditions introduce questions of **configurational averaging**, a topic of ongoing study.

References

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[6] Ziegler, Ziegler, Biersack, Nuc. Inst. and Meth. in Phys. Res., **268**, (2010)

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