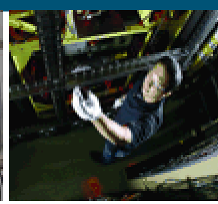
SAND2018-2282C

First-principles Stopping Power in Warm Dense Matter



PRESENTED BY

Attila Cangi, Daniel S. Jensen, Andrew D. Baczewski

APS March Meeting, Los Angeles
March 9, 2018
Session Y38: Materials in Extremes: Warm Dense Matter

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

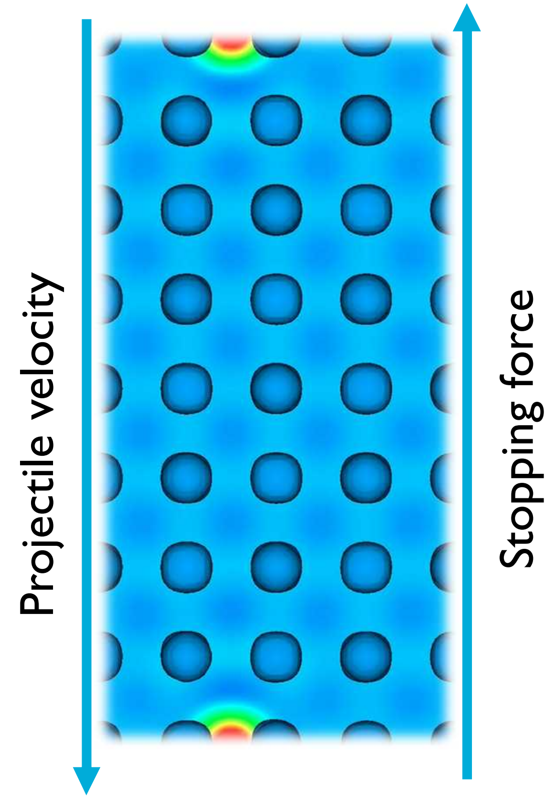
Electronic Stopping in Warm Dense Targets

Stopping mechanisms

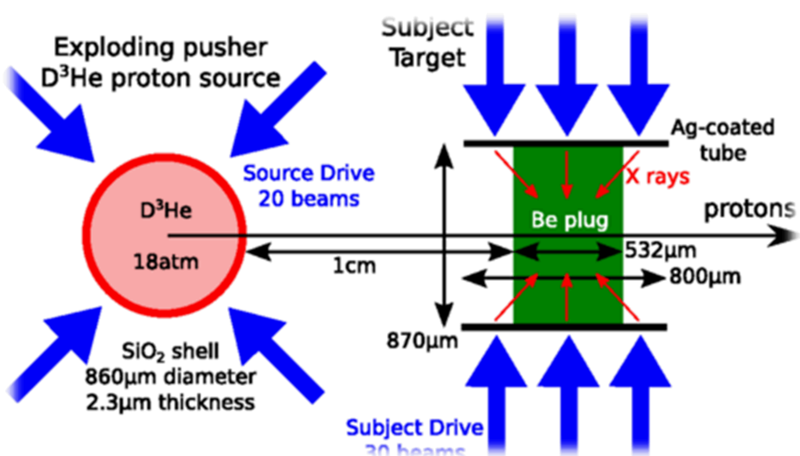
- Nuclear stopping (lattice vibrations)
- Electronic stopping (electronic excitations, quantum effects)

Large body of literature for cold targets

- Empirical approximations (*Rutherford, Thomson, Bohr, Bethe*)
- Parameter-free atomistic simulations
  - Electronic structure coupled to molecular dynamics
  - Cold stopping power (*Echenique, Correa, Artacho, Schleife*)



$$\frac{\partial E}{\partial s} = \frac{1}{v}\frac{\partial}{\partial t}\left\langle \frac{\mathbf{P}^2}{2M} \right\rangle$$



Zylstra et al., Phys. Rev. Lett. **114**, 215002 (2015).

Sandia's Capability: TDDFT for Warm Dense Matter

Sandia implementation of TDDFT-Ehrenfest MD in VASP

- Andrew D. Baczewski et al., PRL **116**, 115004 (2016)
- Plane wave basis
- Projector-augmented wave (PAW) formalism
- Crank-Nicolson time integration (unitary)
- Generalized minimal residual method

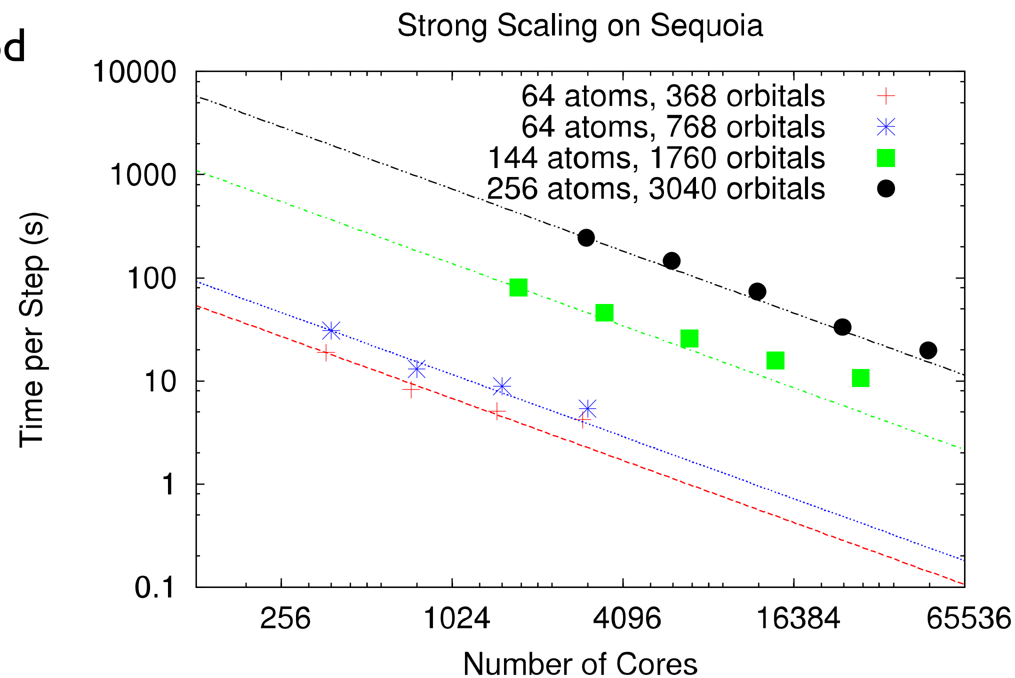
$$i\frac{\partial}{\partial t}\phi_i(\mathbf{r},t) = \left\{-\frac{1}{2}\nabla^2 + v_{\mathrm{S}}(\mathbf{r},t)\right\}\phi_i(\mathbf{r},t)$$

$$M_\alpha\frac{\partial^2\mathbf{R}_\alpha}{\partial t^2} = -\nabla_{R_\alpha}E[R_\alpha, n(\mathbf{r},t)]$$

$$\vec{F}_\alpha = \sum_{nqq'} f_n\mathbf{C}^*_{nq'}(t)\left[\nabla_{R_\alpha}\mathbf{H}_{\mathrm{S}} - \epsilon_n\mathbf{S}\right]\mathbf{C}_{nq}(t)$$

Scales well on DOE machines

- Typically 100s of cores, a few hours
- No "free" parameters
  - takes mass density
  - # of electrons
  - exchange-correlation functional

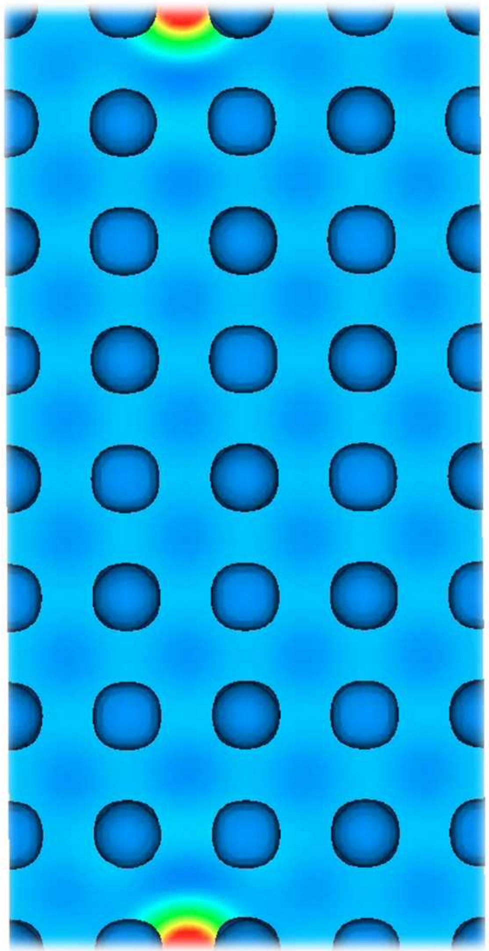


Born-Oppenheimer Fails: Importance of Non-Adiabatic Effects

Hydroge moving through cold, bulk aluminum in a channeling trajectory

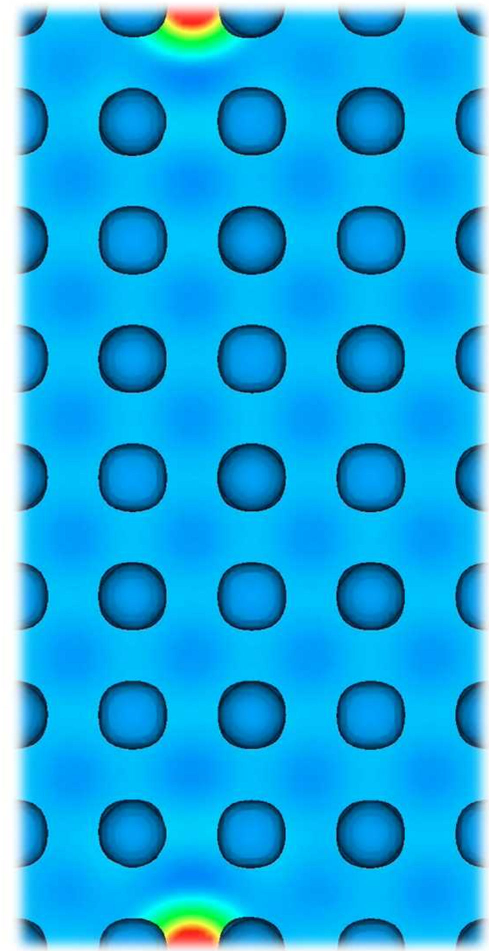
Born-Oppenheimer MD

Projectile velocity



No stopping power (unphysical)

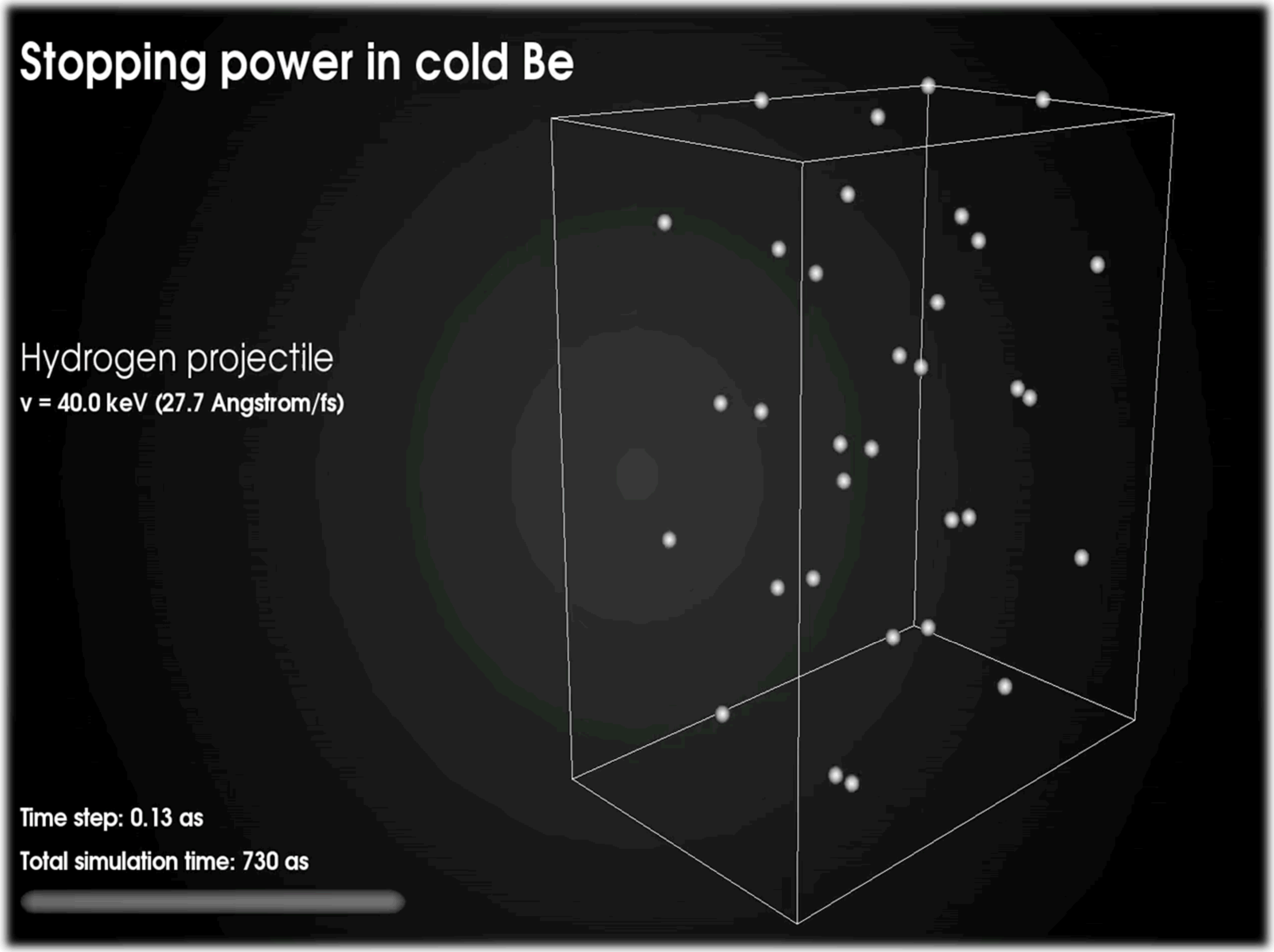
Ehrenfest MD



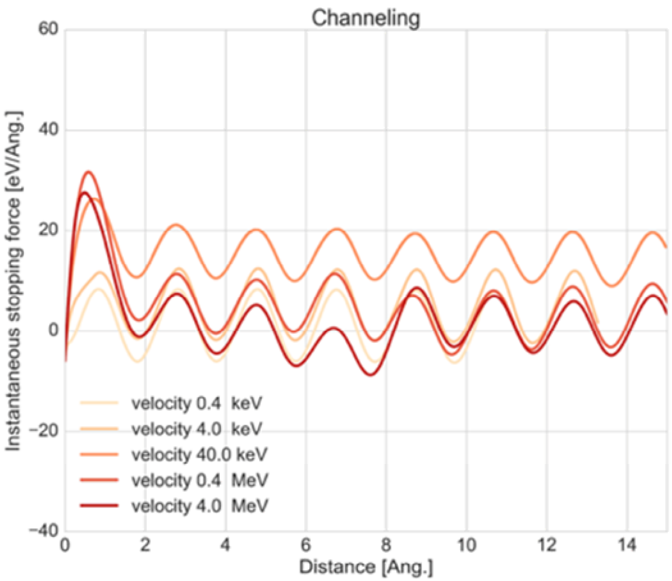
Stopping force

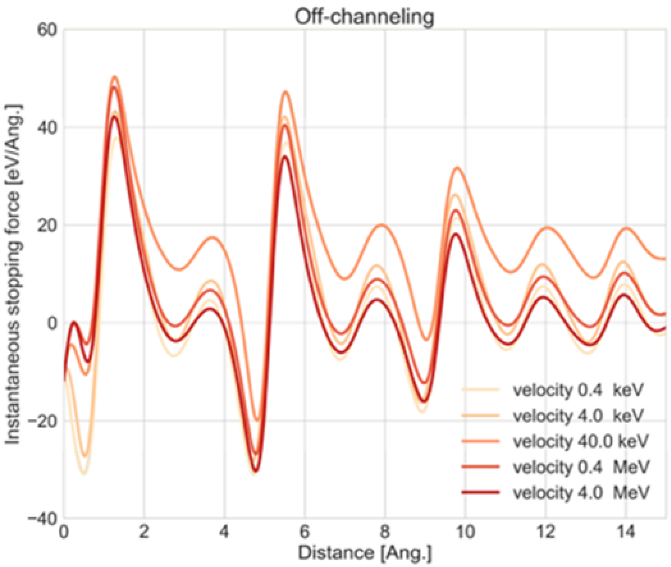
Matches experimental stopping power

H/Be Stopping Simulation

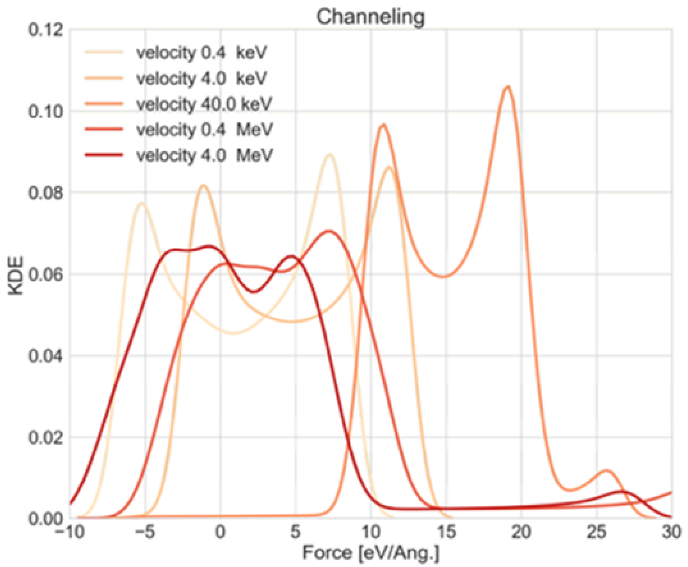


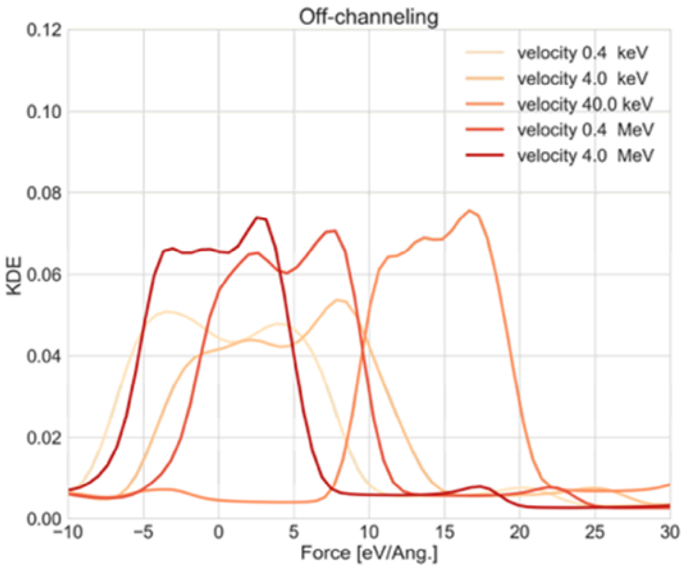
Electronic Stopping Force



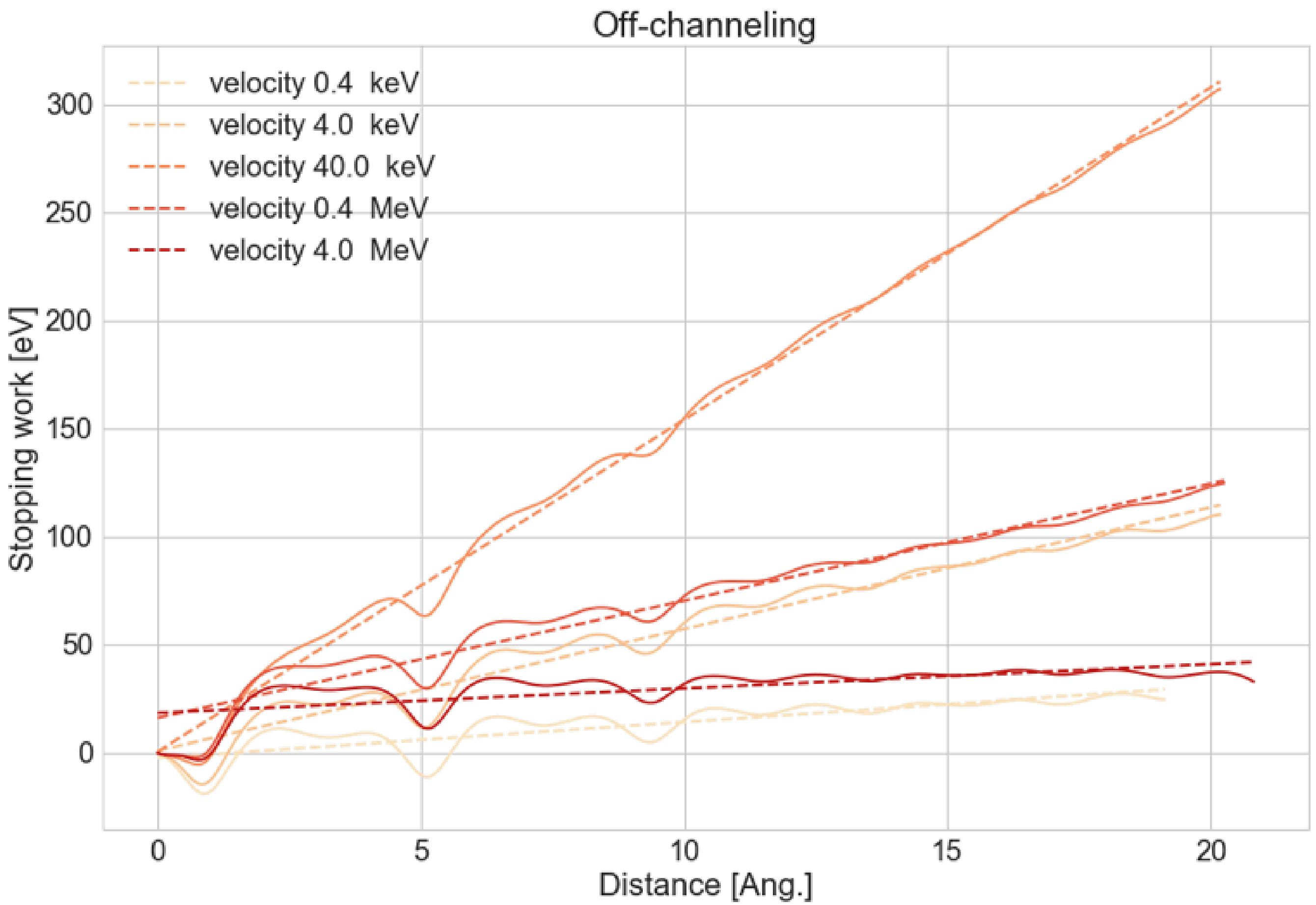


Statistics of the Electronic Stopping Force



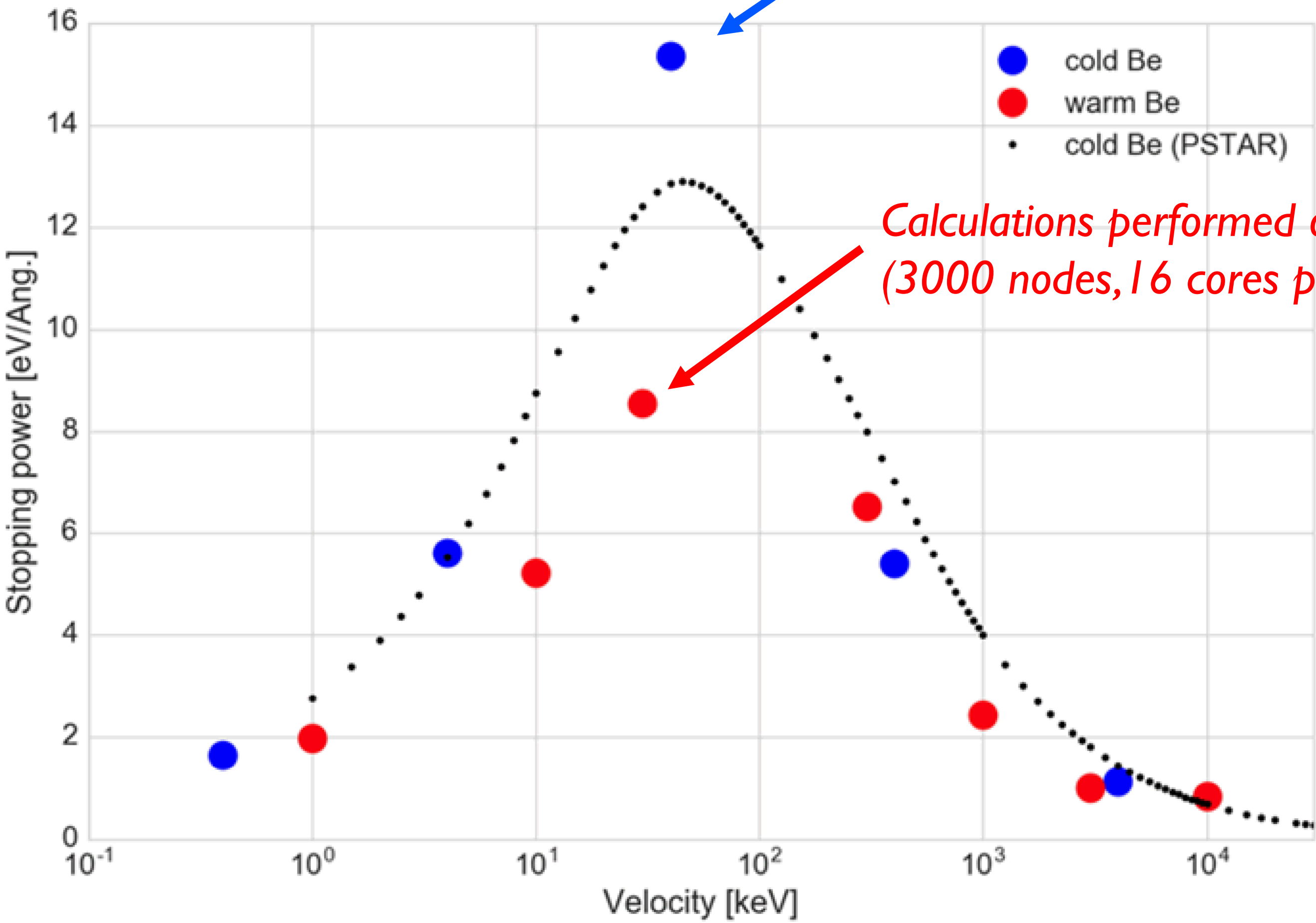


Electronic Stopping Work



Electronic Stopping Power

Calculations performed on ***Solo***
(5 nodes, 32 cores per node, 1 day)



Calculations performed on ***Sequoia***
(3000 nodes,16 cores per node, 1 day)

Conclusions and Future Work

First-principle stopping power calculations help constrain experiments and lower level methods (empirical formulas).

Capability to improve databases of stopping curves for a wide range of warm dense targets

- Mixtures of target materials
- Different types of projectiles
- Collect statistical data

Future developments

- **Computational efficiency**
  - Stopping power from TDDFT on average-atom models
- Accuracy
  - More accurate inclusion of non-adiabatic effects from exact factorization method
  - Methods beyond TDDFT (non-equilibrium many-body perturbation theory)