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Elestronic stopping of ionic projectiles in ice and metals

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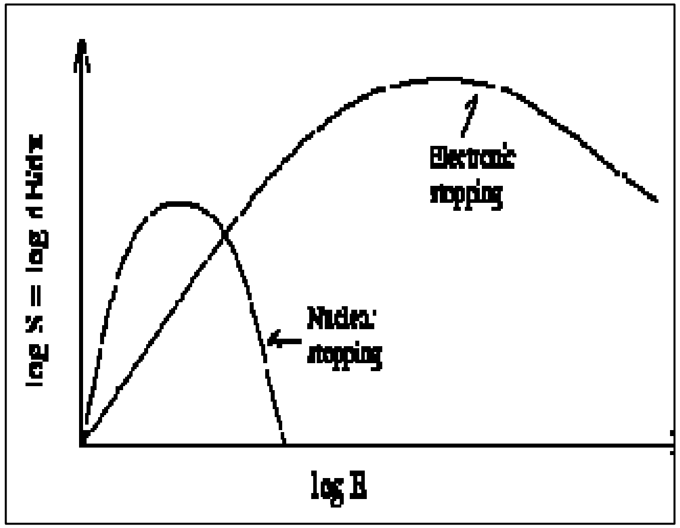
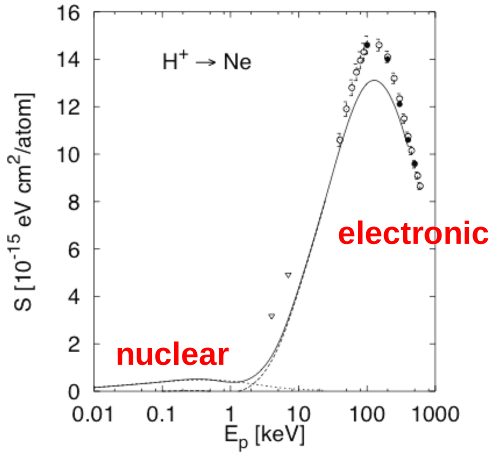
Ionic projectiles

Ionic projectiles
electronic vs nuclear stopping

- Stopping power: energy deposited per unit length (S=dE/dx)
  - **Nuclear**: dominates at low energies
  - **Electronic**:
    - **Metals**: for v→0, S ~ v (e-h pairs). Decrease a large v (Bethe)
    - **Insulators**: Threshold due to band gap $v_{th} \approx$ 0.1–0.2 a.u.

      [First-principles on LiF: M. Pruneda et al., Phys. Rev. Lett. **99**, 235501 (2007)]





Schiefermuller et al., Phys. Rev. A **48**, 4467 (1993)

Cabrera-Trujillo et al., Phys. Rev. Lett. **84**, 5300 (2000)

Ionic projectiles

Regions of interest for biomolecular systems

- Water is an electronic insulator -- E_g (water) ~ 10 eV.
  - Threshold effects separate nuclear from electronic stopping. Low and high energy regimes can be treated separately
    - **Low energy (v < 0.1 a.u., or 4 keV for C): <u>adiabatic regime</u> (GS electrons)**
    - **High energy (v > 0.1 a.u.): <u>sudden regime</u> (purely electronic dynamics)**
- Depending on the energy levels of the projectile:
  - Electronic excitation, capture and ionization by low-energy ions is possible.
    - **Intermediate energy: impact fragmentation coexists with electronic excitation. <u>Combined electron-nuclear dynamics required</u>.**

Computational methods

Real-time electronic dynamics

- **Sudden regime**
  - **Real-time electronic dynamics** via **TDDFT**
  - Adiabatic GGA (**AGGA**) approximation to time-dependent XC
  - **Fixed nuclei**
  - Incident ion treated as a **moving external potential**
  - **Channeling** to avoid direct impact

- **Time-dependent Kohn-Sham equations implemented in SIESTA**
- [A. Tsolakidis, D. Sanchez-Portal and R. M. Martin, Phys. Rev. B 66, 235416 (2002)]

$$i\hbar \frac{\partial \Psi_i^{KS}}{\partial t} = H\Psi_i^{KS}$$

with Kohn-Sham orbitals expanded in atomic orbital basis

$$\Psi_i^{KS}(r,t) = \sum_{\mu} c_i^{\mu}(t)\phi_{\mu}(r)$$

$$i\hbar \frac{\partial \mathbf{c}}{\partial t} = \mathbf{S}^{-1}\mathbf{H}\mathbf{c}$$

Computational methods

Ehrenfest dynamics

- **<u>Sudden regime</u>**
  - **Real-time electronic dynamics** via **TDDFT**
  - Adiabatic GGA (**AGGA**) approximation to time-dependent XC
  - **Classical MD for the nuclei**
  - Incident ion treated as **another classical particle**
  - **No channeling restrictions**

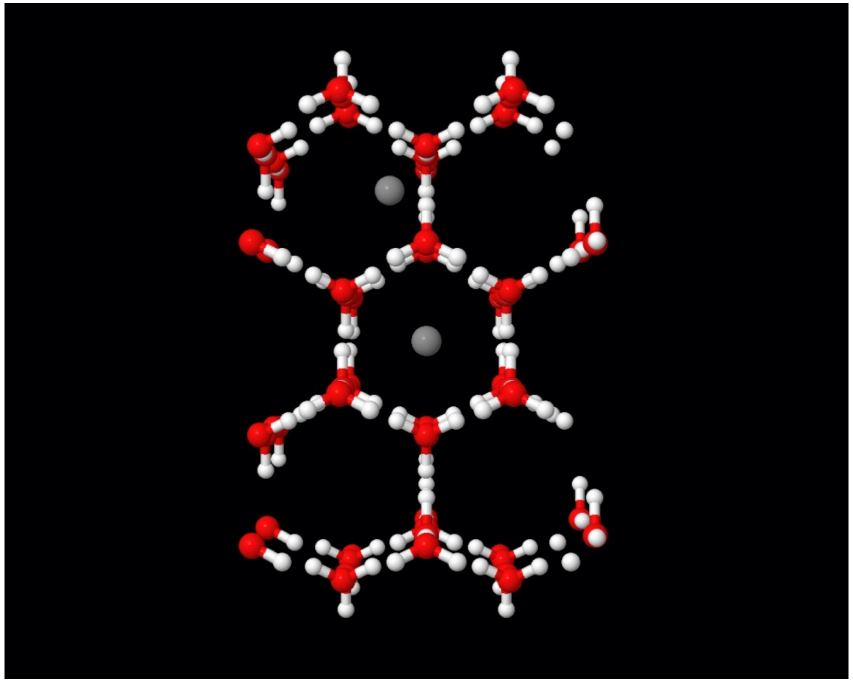
- **Ehrenfest equations implemented into SIESTA**

  [D. Sanchez-Portal, J. Kohanoff and E. Artacho (unpublished)]

Leap-frog
Crank-Nic.
Projections

Electronic stopping in ice

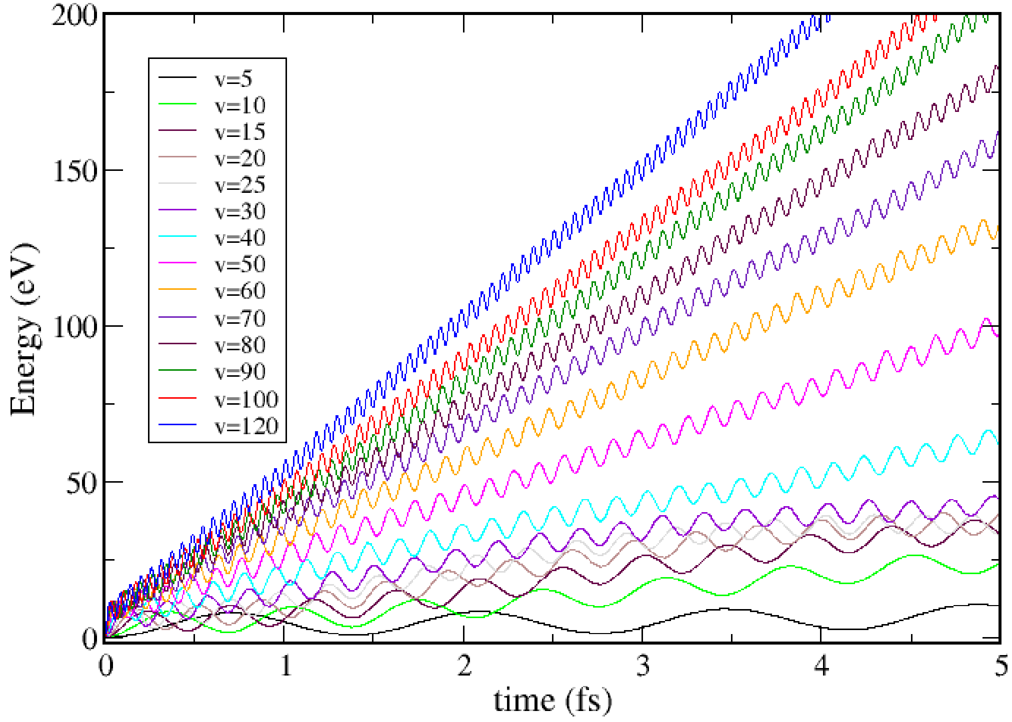
H+ shooting through channels in hexagonal ice
(24 and 40 water molecules – 3 and 5 units)

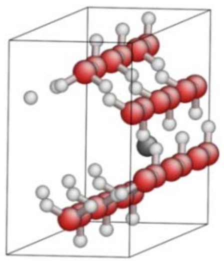


Non-adiabatic stopping

channeling of H^+ through hexagonal ice

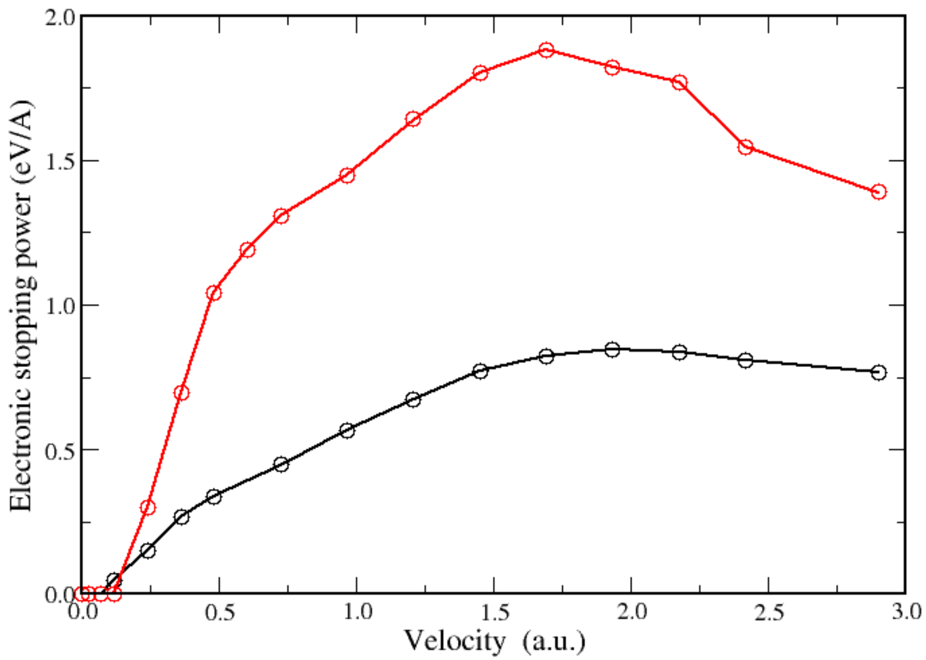
Energy transferred to electrons





Electronic stopping power

channeling of H^+ through hexagonal ice



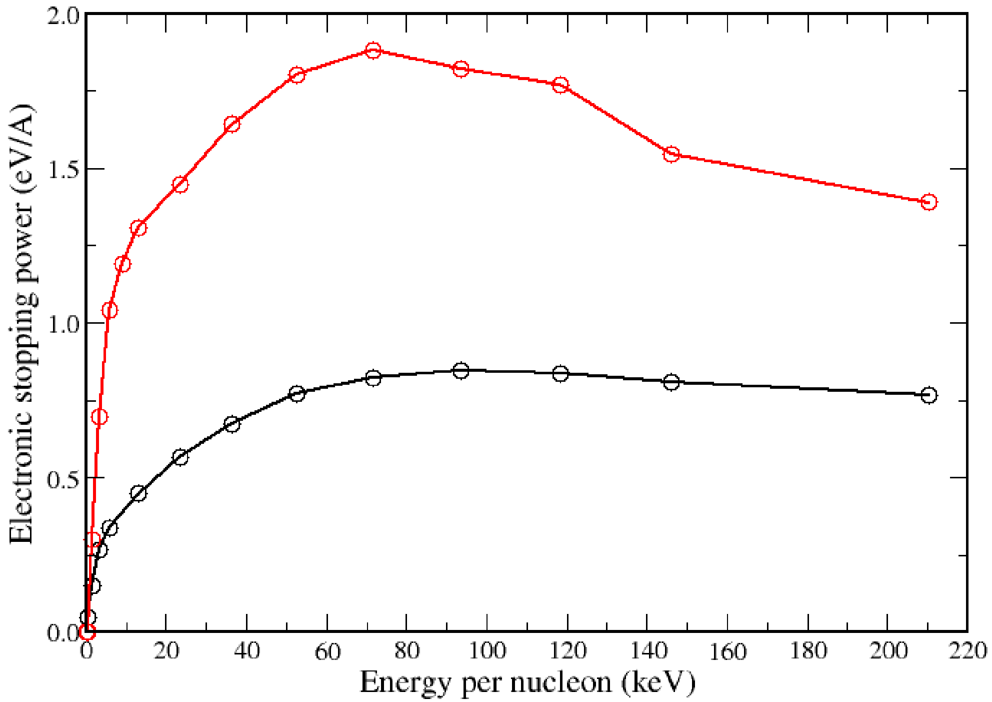
- S_e through center of channel is about half that of LiF
- Channels in ice are more open
- S_e increases by a factor of 3 when proton travels closer to water molecules

Electronic stopping power

channeling of H^+ through hexagonal ice

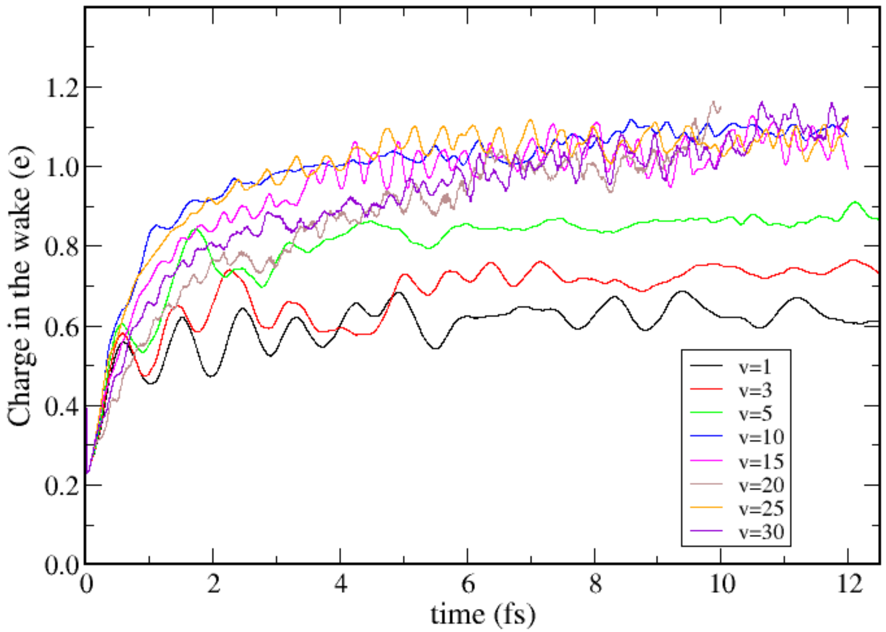
Experiment: P. Bauer et al., NIMB 93, 132 (1994)

Peak at 90 keV/nucleon



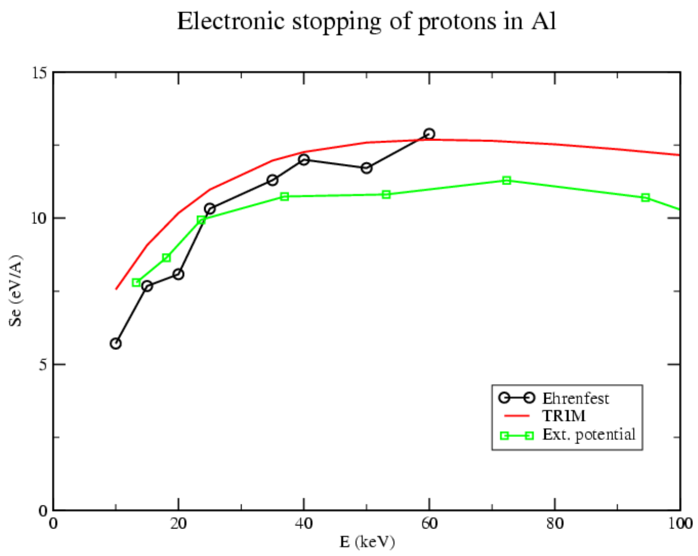
Non-adiabatic stopping

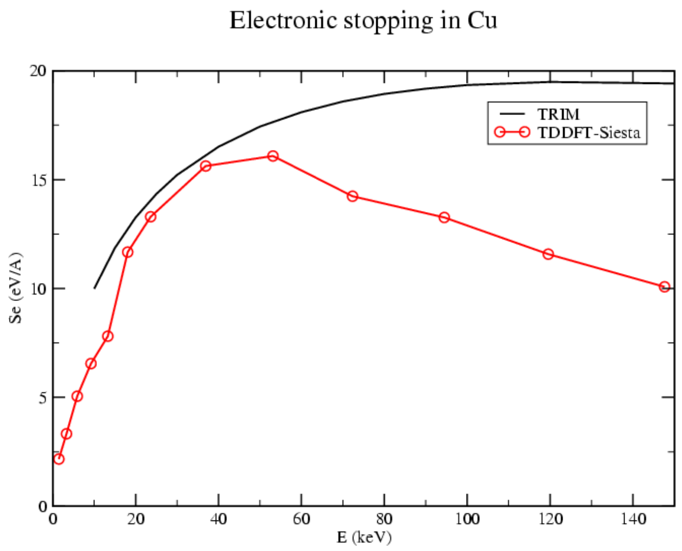
Charge state of the proton

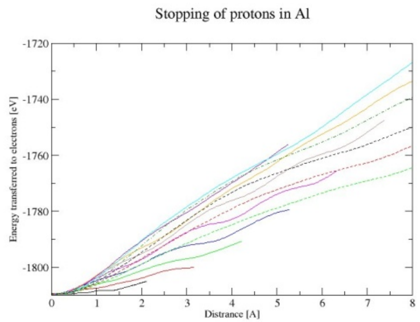


- At low speed the proton drags the electronic charge with it, forming H.
- At higher speed, electrons respond to the proton, but too late, creating a wake.
- Eventually, the electronic wake detaches and the proton travels as H^+.

Electronic stopping in metals

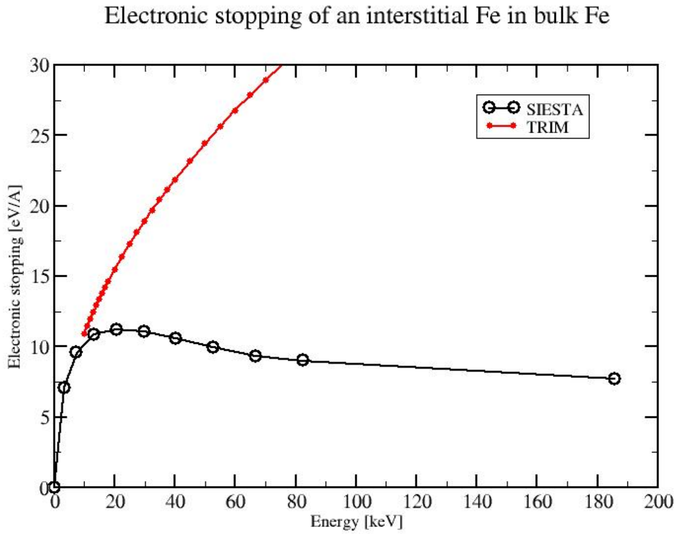


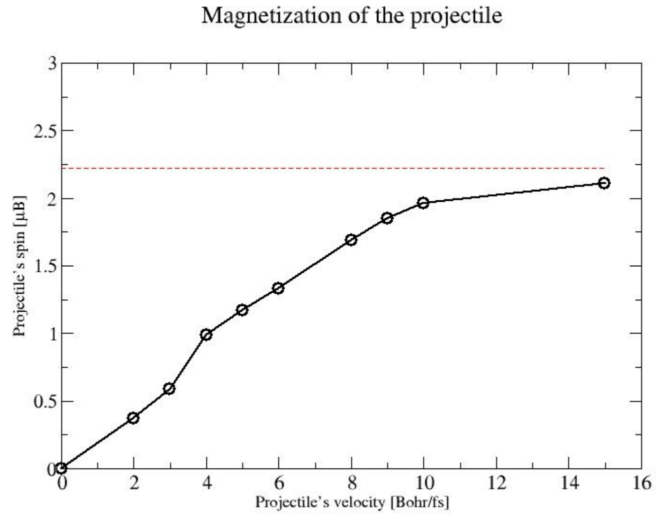


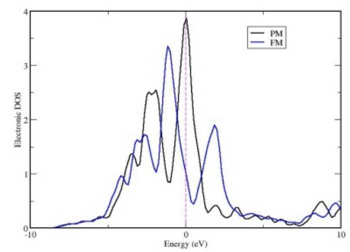


SRIM stopping tables reproduced !

Nuclear materials: stopping of Fe in Fe







It is possible to compute S_e for heavier projectiles

FM vs PM: influence of EDOS apart from ρ