Ab initio electronic stopping in efficient atomistic simulations

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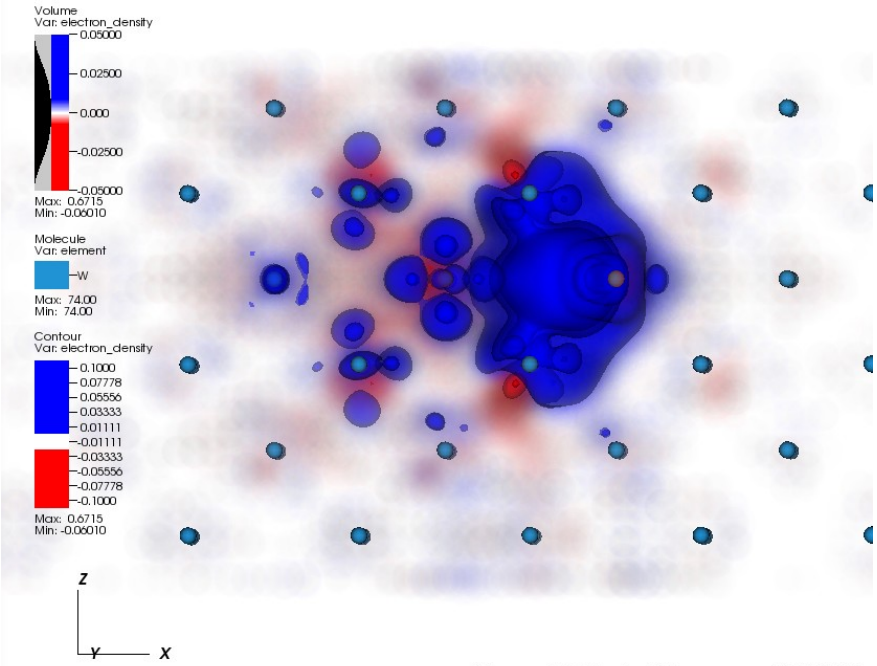
Environmentally dependent energy dissipation

- TD-DFT can capture dynamic energy losses in any local environment
- Questions: validity of various approximations used
  - Adiabatic LDA
  - Core electrons
  - Basis sets
- *Though the calculation is* ab initio, *we still need experimental confirmation!*

Electron density change (W in W) (1.14MeV v = 0.5 at.u.)



Sand/Ullah/Correa (2018)

MDRANGE

- MD-based method
  - Many-body interactions
  - Only projectile-target interactions
  - Only small part of target followed at a given time
- Include electronic stopping
- Different repulsive potentials
- Sputtering and implantation simulations