SIMUNE
ATOMISTIC SIMULATIONS

## CASE STUDY –RADIATION DAMAGE

# Electronic stopping power in a narrow band gap semiconductor from first principles

Ullah, R. Corsetti, F. and Sánchez-Portal and E. Artacho, Phys. Rev. B., 91, 12520 (2015)

Motivation of the modeling: The study of fast-moving charged particles shooting through solid materials is of great interest from the point of view of applications ranging from nuclear engineering to biological soft matter for medical applications and material engineering for space electronics. Experimentally it is almost impossible to measure directly electronic stopping power (ESP) at low velocities (< 0.2 a.u.), whereas in simulations it is possible to directly access the ESP.

Achievements of the model: The direction and impact parameter dependence of electronic stopping power, along with its velocity threshold behavior, is described for a prototypical small band gap semiconductor. The distinct velocity threshold observed in experiments is well reproduced, and its non-trivial relation with the band gap is found to follow a perturbation theory argument.

Model system/Software: The ESP of H in Ge is investigated. The calculations are carried out using an extension of the **SIESTA** program and method which incorporates time-evolving TD-DFT based non-adiabatic electron dynamics simulations.

The following key issues were investigated:

- description of ESP in different crystal directions
- dependence on direction and impact parameter of ESP for projectile velocities ranging from 0.05 to 0.6 atomic units
- reproduction of the distinct velocity threshold observed in experiments

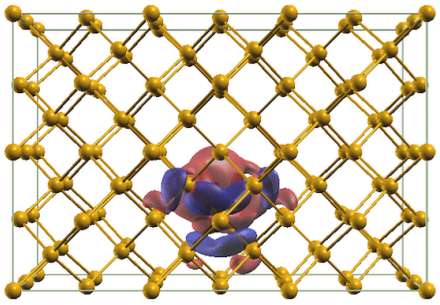

Figure: Schematic representation of the static screening of a H projectile in the [001] direction of a Ge crystal. Figure created by Ullah R, author of Phys. Rev. B., 91, 12520 (2015)

**Emilio Artacho**, part of the SIMUNE´s board of experts and member of the core development team of the SIESTA code, is one of the authors of this work.