**XXIII Simposio Chileno de Física**
Chile, 22-24 noviembre 2022 Materia Condensada y Física del Estado Sólido

# Stopping coefficients of slow light ions. A density functional theory approach

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## Abstract

We present a density functional theory (DFT) approach to study the stopping coefficient $Q$ for hydrogen, helium and lithium ions at the low velocity limit. An electron gas is used to represent the conduction or valence electrons of the target. The interaction of external charged particles with the free electrons of a material is a problem of relevance for numerous studies dealing with impurities in solids, radiation effects and materials analysis. Particularly, today hydrogen and lithium is widely used in the industry to manufacture batteries for different electrical devices. A remarkable aspect of the DFT is that the quantum mechanical problem of determining the equilibrium state of a many-body system may be solved if the ground state density of the electrons is found. Then the self-consistent solution yields the phase shifts as a function of the electron speed (or electron energy). In this work are calculated as a function of the electronic density $n_e$ the most representative terms that characterize the interaction of an external charge with a free-electron gas: the scattering phase shifts $\delta_l(v_e)$ and the corresponding stopping coefficient, where $v_e$ is the electron speed. Using the values so obtained we calculate the transport cross section $\sigma_{tr}$ by [1]

$$\sigma_{tr} = \frac{4\pi}{v_F^2} \sum_{l=0}^{\infty} (l+1) sin^2[\delta_l(v_F) - \delta_{l+1}(v_F)], \tag{1}$$

here $v_F$ is the Fermi velocity. If $v$ is the ion velocity, we determine the stopping coefficient $Q \equiv -\frac{1}{v}\frac{dE}{dx}$ using the relation [2,3,4]

$$Q = n_e m v_F \sigma_{tr}, \tag{2}$$

where $m$ is the mass of the ion. Results are compared with experimental data obtained in different solids by other autors [5].

### References

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