Electronic stopping of particles in matter: anomalies for slow antiprotons in LiF

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There has been significant progress in the first-principles simulation of the non-equilibrium electronic processes triggered by energetic particles traversing matter. The electronic stopping power (ESP) gives the rate of energy transfer from the projectile motion to target electrons, which can reach scales of eV/Å to keV/Å, quite removed from linear-response descriptions of dynamical processes. Real-time time-dependent density-functional simulations have proven to be quite quantitative in their description, giving us some confidence in the predictive power of the technique. Such first-principles calculations have recently challenged two fundamental tenets in the field. It is quite generally accepted that (i) ESP is larger for positively charged projectiles than for their negative antiparticles, and (ii) insulators display a velocity threshold below which ESP is negligible. Recent first-principles calculations of ESP for protons and antiprotons in LiF [1] seem to find exception to both propositions: the threshold seems effectively to disappear for antiprotons while remaining well defined for protons, the latter fact being consistent with experiments. In our own first-principles calculations, we reproduce their results in the same [111] off-center channelling conditions they used. We explain the phenomenon by a mid-gap level appearing for antiprotons, which effectively oscillates approaching the conduction band as the antiproton moves, fitting well to an elevator effect [2]. However, we find that the effect disappears for other directions of propagation, and washes out when averaging, recovering both the threshold and the expected Barkas effect, and therefore predicting an important sensitivity of ESP to experimental setup (unidirectional controlled channelling vs otherwise) for low velocities.

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[1] X. Qi, F. Bruneval and I. Maliyov, Phys. Rev. Lett. **128**, 043401 (2022).

[2] A. Lim, W. M. C. Foulkes, A. P. Horsfield, D. R. Mason, A. Schleife, E. W. Draeger, and A. A. Correa, Phys. Rev. Lett. **116**, 043201 (2016).