Laboratório de Implantação Iônica
Instituto de Física - UFRGS

44 anos

Ion Implantation Laboratory
Institute of Physics - UFRGS

Biennial Report - 2023/24

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Editors
Henrique Trombini
Silma Alberton Corrêa
Pedro Luis Grande

Porto Alegre

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Editores:

Henrique Trombini - docente da Universidade Federal de Ciências da Saúde de Porto Alegre (UFCSPA).

Silma Alberton Corrêa - docente da Universidade Federal do Rio Grande do Sul (UFRGS) do Instituto de Química, no Departamento de Físico-Química.

Pedro Luis Grande - docente da Universidade Federal do Rio Grande do Sul (UFRGS) do Instituto de Física, no Departamento de Física.

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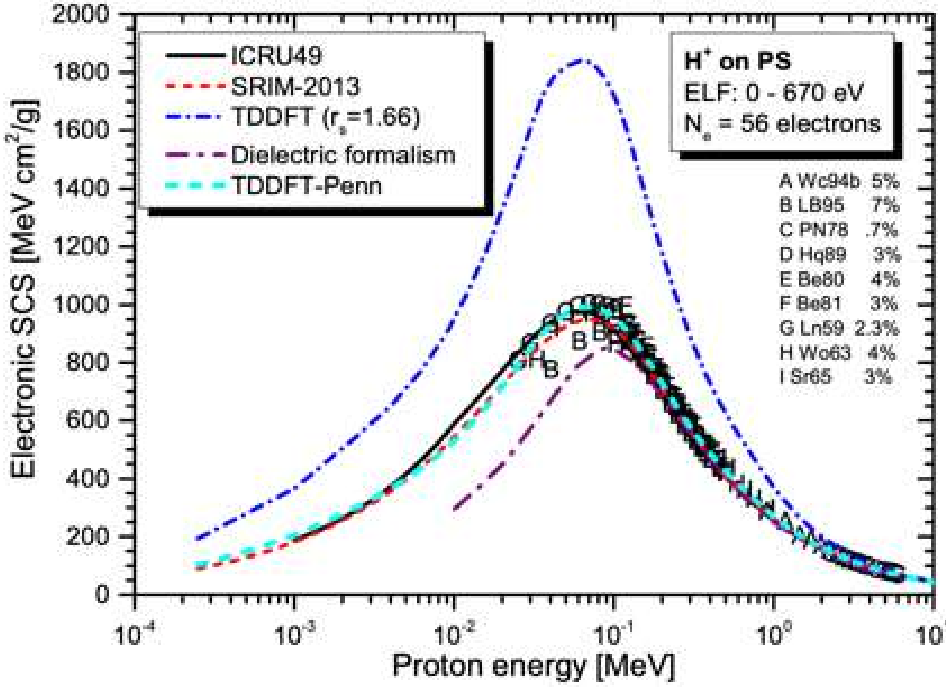
Efficient computational modeling of electronic stopping power of organic polymers for proton therapy optimization

Pedro Luis Grande

This comprehensive study investigates the interaction of protons with organic polymers, focusing on the spatial electron density distribution's impact on stopping power estimates. The study refutes the common assumption of homogenous electron density in polymers, revealing that this overestimates stopping power values at energies below 2 MeV. Employing real-time time-dependent density functional theory (TDDFT) coupled with the Penn method, researchers developed a real-time TDDFT-Penn theoretical framework to model electronic stopping power across a wide energy range accurately. The study highlights that precise modeling of materials with complex electronic structures is critical for applications like proton therapy.

The Bragg rule, commonly used to calculate stopping values for compounds, exhibited significant deviations from experimental data around the stopping maximum, particularly in polymers like PMMA and PI. These deviations are attributed to the complex molecular structures and potential charge transfer effects due to varying electronegativities in the bonds of these polymers. The breakdown of the Bragg rule impacts the predicted mean excitation energies and projectile range, underscoring the need for more accurate models that account for the intricate electronic structures of polymers. The study concludes that the real-time TDDFT-Penn approach offers a physically sound and precise method to model electronic stopping power in polymers, improving our understanding of ion-polymer interactions and paving the way for advancements in proton therapy and other fields.



Proton SCS in PS polymer. Real-time TDDFT results using a unique FEG (r_s =1.66 au) and real-time TDDFT-Penn. Experimental data (uppercase letters) concentrated around the stopping maximum. Dielectric formalism results in purple dash-dot - line. Semi-empirical models - ICRU49 and SRIM-2013 showcased.

Paper reference:

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