

# Inelastic collision calculations of heavy targets

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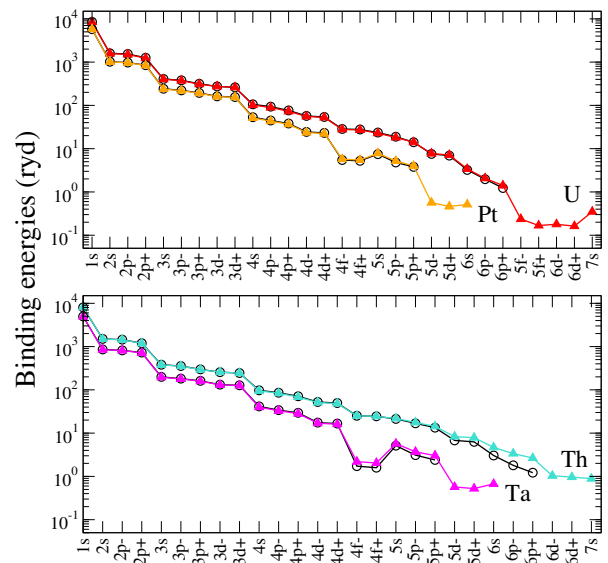
Fully relativistic structure calculations for a series of heavy targets are presented here. The description of these atoms requires the solution of the relativistic Dirac equation. We used the HULLAC suite of codes to compute their atomic structure. The results obtained for the energies of the bound orbitals are compared with experimental ones, obtaining a good overall agreement. The method uses the parametric potential model that allows to obtain a unique potential. This enable us to represent both bound and continuum states in the same footing, which is of great interest in several inelastic collisional calculations. We computed energy loss and L-shell ionization for these relativistic atoms, showing good agreement with experimental results.

The description of heavy atoms requires the solution of the relativistic Dirac equation. To this end, we used the HULLAC code package [1], which allows one to obtain accurate relativistic one-electron orbitals and multiconfiguration bound states and energies. The calculations are based on first-order perturbation theory with a central field, including the contribution from the Breit interaction and quantum electrodynamics corrections. The detailed energy levels are computed using the RELAC code [2], which uses the parametric potential model. This model consists in minimizing the first-order relativistic energy of a given set of configurations for a parametric analytical function for the screening charge distribution. Although this code was written for calculations of heavy ionized atoms, it can be successfully employed in other atomic systems, such as the ones presented here.

The binding energies obtained for Ta, Pt, Th and U ( $Z=73, 78, 90, 92$ ) using the fully relativistic method are shown with up-filled triangles in Fig. 1. The figure also includes experimental bound energies [4] (hollow circles). The values computed for the inner orbitals agree with the experimental ones in about 2%. The discrepancies found with the more external shells are accounted for the structure differences between the atoms (computed) and the solids (experiments).

The relativistic atomic structure calculated were used to compute inelastic collisional processes, such as energy loss, straggling and L-shell ionization. In previous work, structure calculations were performed to describe energy-loss and straggling of W, Au, Pb and Bi ( $Z=74, 79, 82, 83$ ) [5] for protons. L-shell ionization calculations of these heavy atoms were also made in several theoretical approaches, showing very good

agreement with experimental results [6].



**Figure 1.** Theoretical and experimental binding energies for Pt, U, Ta, and Th.

## References

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