Energy loss of charges interacting with metallic nanoparticles

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A STRACT

e present a study on the interaction of moving charged particles with metal clusters and nanoshells.

First, we make use of time-dependent density functional theory TDDFT to calculate the energy lost by antiprotons colliding through the center of spherical jellium clusters of different size and electronic density parameter r_s. The results allow us to define an effective stopping power as the energy loss per unit path length inside the cluster.

Analysing the dependence of on the projectile velocity, we obtain a result which is unexpectedly close to the one corresponding to the free electron gas, even for very small clusters and low velocities. e conclude that the collision process is quite local, and that the discreteness of electronic states in the cluster does not play an important role in the screening process.

oreover, the stopping powers obtained from our calculations using nanostructures of a few nanometeres in size are comparable to experimental values for macroscopic materials, both for protons and antiprotons. This reassures us that the dynamic screening within the cluster is essentially that of a homogeneous system in the velocity range considered.

For completion of the study, we also show the velocity dependence of in collision processes with off-center projectile trajectories, as well as the case of the interaction of antiprotons with nanoshells of different electronic density parameters and size.

THEORETICAL AC ROUND

-spherical jellium cluster $N = (R_{cl}/r_s)^3$

-time-dependent density functional theory TDDFT

$$i\frac{\partial \psi_j(\mathbf{r},t)}{\partial t} = \{T + V_{\rm ext}(\mathbf{r},t) + V_{\rm H}(\mathbf{r},t) + V_{\rm xc}(\mathbf{r},t)\}\,\psi_j(\mathbf{r},t)$$

-external potential created by moving projectile

$$V_{\rm ext}(\mathbf{r},t) = Q/[|\mathbf{r}-\mathbf{R}(t)|], \qquad \mathbf{R}(t) = \mathbf{R}_0 + \mathbf{v}t$$

-force on the projectile

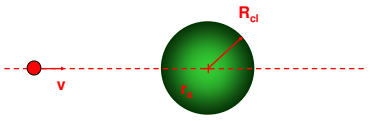
$$\mathbf{F}[\mathbf{R}(t)] = -Q\int d^3\mathbf{r}'\,\frac{[n(\mathbf{r}',t) - n_0^+(\mathbf{r}')]}{|\mathbf{R}(t)-\mathbf{r}'|}\,[\mathbf{R}(t)-\mathbf{r}']$$

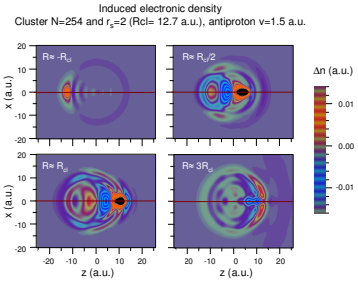
-energy loss in the collision process

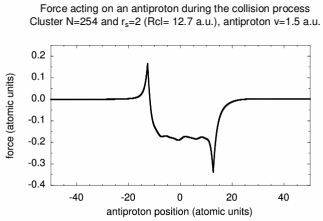
$$\Delta E = v\int_{-\infty}^{\infty} F_z(t)dt \qquad \Delta E = -[E_{\rm el}(t\to\infty) - E_{\rm el}(t=0)]$$

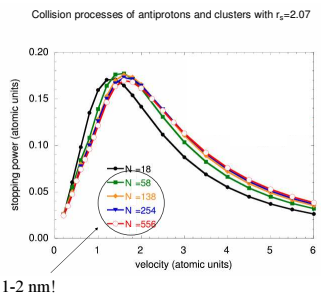
-effective stopping power $S = \Delta E/(2R_{\rm cl})$

ANTIPROTON AND PROTON COLLISIONS WITH CLUSTERS

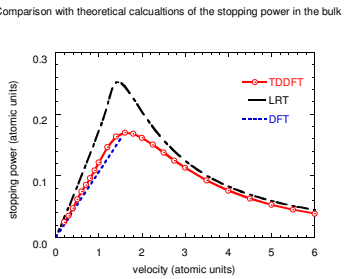


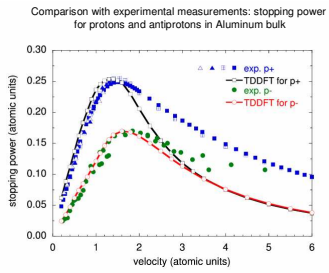






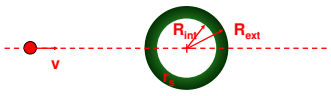
N	R_{cl}(a.u.)
18	5.42
58	8.01
138	10.70
254	13.11
556	17.02

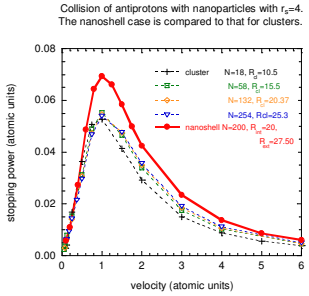




Reference: M. Quijada, A.G. Borisov, I. Nagy, R. Díez Muiño and P.M. Echenique, *Physical Review A* **75**, 042902 (2007)

ANTIPROTON COLLISIONS WITH NANOSHELLS





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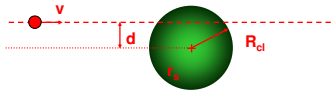

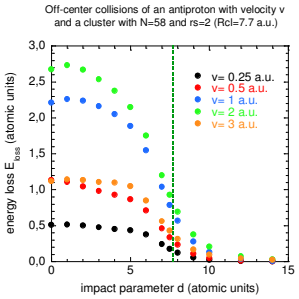

CONCLUSIONS

-Our TDDFT calculations reproduce stopping powers for bulk systems in the well-known limits of low- and high-velocity projectiles

-The average stopping power of metal nanoparticles for charged probes is independent on the particle size over a wide range of velocities, even for systems of less than a nanometer in size.

-The calculated values of the stopping power of metal nanoparticles agree quantitatively with recent experimental measurements in Aluminum.

-Finite sized systems can be used to study the energy loss of charged projectiles moving inside metallic solids.