

Supplementary material for: Laser Induced Electron Diffraction for Probing Rare Gas Atoms

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Detailed comparison on e -neutral-atom and e -ion scattering cross sections

In Fig. 2 of the main text, we compared the e -neutral and e -ionic scattering differential cross sections (DCS) in linear scale for Ar and Kr at 150 eV, and Xe at 50eV, respectively. For Xe, its scattering cross section covers 2 orders of magnitude, therefore the comparison for Xe in Fig. 2 is significantly dominated by the large DCS part, i.e., at scattering angles near 180° and 30° . It was stated in the main text that the two theoretical DCS's for e -Xe and e -Xe⁺ do not match in the small angular region, but that is not clearly visible in the linear plot shown in Fig. 2. Here we replot Fig. 2 on logarithmic scale, as shown by Fig. S1. It clearly shows large discrepancy for angular range $[30^\circ, 100^\circ]$ for Xe. For Ar and Kr, the agreement still looks very good on the logarithmic scale, see Fig. S1(a,b). Due to the different angular resolution, the difference near the minima tends to appear larger. Fig. S1(c) shows that the angular range where the DCS between e -neutral and e -ion collisions coincide is more limited at smaller collision energies.

The genetic algorithm fitting procedure

To reconstruct the effective charge distribution $Z(r)$, we parameterized the e -atomic-ion interaction in the form of Eq. (2), with six parameters $\mathbf{a} = \{a_1, a_2, a_3, a_4, a_5, a_6\}$ to be optimized. The fitness function is defined as,

$$\chi^2(\mathbf{a}) = \sum_i [\sigma^{exp't}(\theta_r^i) - \beta \sigma^{theory}(\theta_r^i; \mathbf{a})]^2, \quad (S1)$$

where i the index of the grid points of scattering angle θ , $\sigma^{theory}(\theta_r)$ is the calculated scattering differential cross section (DCS) from each candidate potential $V(r; \mathbf{a})$, and $\sigma^{exp't}(\theta_r)$ is the extracted DCS from the experimental high-energy photoelectron spectra. Since $\sigma^{exp't}(\theta_r)$ is not absolute, a normalization constant is needed to compare absolute theoretical DCS, to search for the best fit. In this work, GA driver GA v1.7a is used, which is implemented by D. L. Carroll in FORTRAN [1]. More details

can be found in Ref. [2].

Calculation of e -ion scattering DCS

The interaction of the electron and the atomic cation is usually modeled by a spherical potential $V(r)$, which consists of a long-range Coulomb potential $V_C(r) = -1/r$ and a local potential $V_s(r)$. The total scattering amplitude for such a potential can be written as

$$f(\theta) = f_C(\theta) + f_s(\theta), \quad (S2)$$

where

$$f_C(\theta) = -\frac{\eta e^{2i\sigma_0}}{2k \sin^2(\theta/2)} \exp\{-i\eta \ln[\sin^2(\theta/2)]\}, \quad (S3)$$

is the Coulomb scattering amplitude with $\eta = -1/k$ and Coulomb phase shift $\sigma_0 = \arg[\Gamma(1 + i\eta)]$. Using partial wave expansion, the scattering amplitude $f_s(\theta)$ is expressed as

$$f_s(\theta) = \sum_{l=0}^{\infty} \frac{2l+1}{k} e^{2i\sigma_l} e^{i\delta_l} \sin \delta_l P_l(\cos \theta), \quad (S4)$$

where δ_l is the phase shift due to short-range potential $V_s(r)$, $\sigma_l = \arg[\Gamma(l+1+i\eta)]$ is the Coulomb phase shift for the l -th partial wave, and $P_l(\cos \theta)$ is Legendre polynomials. As $V_s(r)$ has a finite range, the series in Eq. (S4) usually converges after a certain number of partial waves are added up, and the cutoff partial-wave order l_{max} depends on the electron incident energy. In the case of Ar and Kr, about $l_{max} = 45$ partial waves are needed for scattering energy about 100 eV. From Eq. (S2), we can obtain the scattering cross section $\sigma(\theta) = |f(\theta)|^2$.

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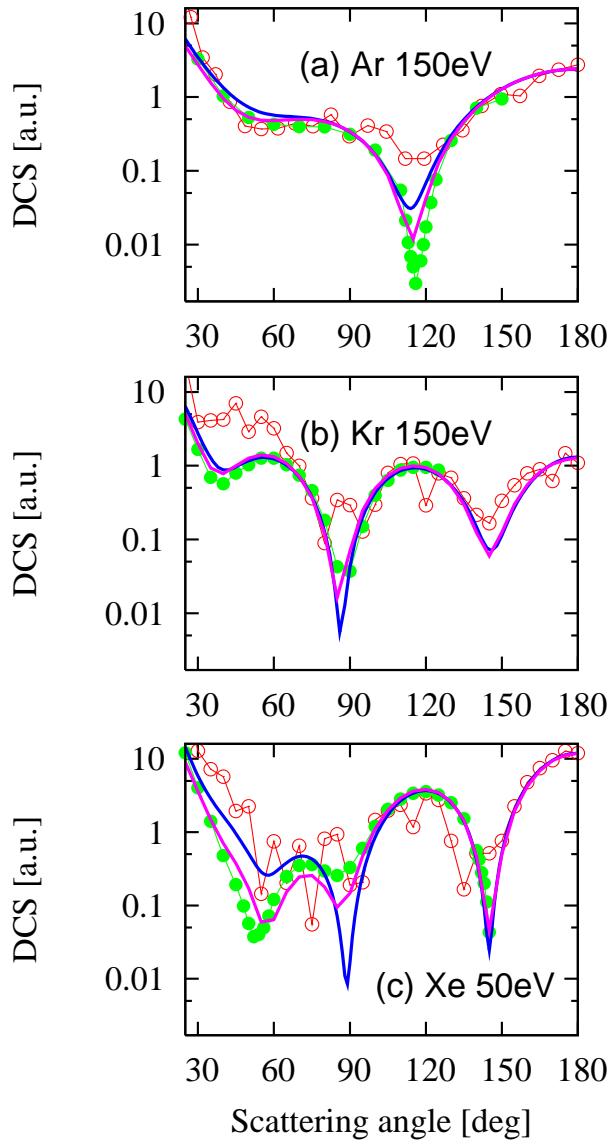


FIG. S1: (Color online) Comparison of e -neutral-atom and e -ion scattering cross section in log scale for Ar, Kr, and Xe at 150, 150, and 50 eV, respectively. DCS from HATI: red empty circles; theory e -ion: blue solid lines; experimental e -neutral: green filled circles; theoretical e -neutral: magenta solid lines.