Response to referee reports
JPHYSB-106014

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We appreciate the comments and questions of the three referees. They were taken into account, as explained in the replies to each referee. In what follows, the referee reports are in black letters and our answers and comments in blue.

Summary of the modifications: The manuscript was changed from letter to regular manuscript by the editorial board. Attending to this fact and the comments by the three referees requesting further explanations, we decided to modify the manuscript by dividing the text into three sections: Introduction, Scaling rules (with subsections), and Conclusions. Additional specifications of the scaling models are given in Section II-A, B, and C. Figure 2 was improved by including a gray area of $\pm 30\%$ that covers most of the available data. Also, experiments for H^+ and He^{+2} in water (missing in the previous version) were added to the figures (Refs. 25, 26, and 27), extending the energy range where the present scaling agrees with the experimental data. Following the suggestion by one of the referees, we changed the title from "Universal scaling for the ionization..." to "Scaling rules for the ionization...".

1 Reply to report of the First Referee

The authors propose the universal scaling law of the ionization cross sections by the impact of multiply charged atomic ions on the basis of the experimental data reported in their very recent publication [J. Phys. B, 53, 055201 (2020)]. Their conclusion of this newly submitted paper is that they found the scaling law of Eq. (1) with the alpha value of 1.2. However, as the authors mention in the introduction part, the same scaling law with the alpha value of 4/3 = 1.333 was reported in 2013 by DuBois et al. [Ref. 15]. The authors should explain if the scaling with alpha = 4/3, which is very close to their value of 1.2, could not explain the experimental data they recorded. If the value of 1.2 is much better than 1.333, the author should explain possible reason why alpha should be 1.2 on the basis of the physical meaning of the parameter alpha.

The value of $\alpha = 1.2$ was found numerically as the best convergence of the CDW-SSM cross sections of the forty collisional systems over the broadest energy range. Our methodology does not rely on the fitting of experimental data. The work considers the scaling of our theoretical results, which is tested afterward with the experimental data. We also noticed that all the maxima of the theoretical cross sections scaled with $\alpha = 1.2$ lay at the same value of $E/Z^{2-\alpha} = E/Z^{0.8}$. In the present version of our manuscript, we modified lines 59-61 to clarify our choice of α.

About the physical meaning of this parameter, the scaling by Janev et al. [14] uses E/Z^1 as abscissa based on the long-distance approximation for the ionization cross sections. Similarly,

DuBois et al. [15] propose $E/Z^{2/3}$. The 2/3 in Ref. [15] was found by trial and error. However, the dependence with $Z^{2/3}$ recalls the Thomas Fermi model for a constant density of electrons around the ion. In either case, both models are approximations, and our numerical proposal of α is located between them.

2 Reply to report of the Second Referee

The authors propose a scaling formula for cross sections for ionization of complex molecules by multiply charged ions. Such cross sections are required, e.g., for estimating radiation damage in biomolecules. A routine ab-initio calculation of such cross sections by quantum methods is beyond reach of the state-of-the-arts methods. In this situation, it is helpful to have semi-empirical scaling formulas for modeling purposes. Thus, the paper is timely and serves a need. It is concise. However, there are some language issues. The paper should eventually be published as a JPB letter after the authors having adequately responded to my detailed points below.

The points 1)-4), 6) and 7) raised by the referee are language corrections. They were all considered and modified in the manuscript where appropriate.

5) page 1, line 53: I do not see how any value for alpha keeps the Z^2/E relationship? $\alpha = 1.2$ results in $Z^{0.8}/E$.

In first order approaches, the ionization cross section σ depends linearly with Z^2/E. This dependence is valid in the first Born approximation, and at high impact energies, σ/Z^2 scales with E for any charged ion. Within this approximation, σ/Z^α will be a function of $Z^{2-\alpha}/E$ for any value of α. At intermediate energy, the linear dependence with Z^2/E no longer holds, so we numerically sought for the value of α that best merges the cross sections for different impinging charges.

8) Figure captions. Both caption should mention that all plots are for alpha=1.2.

Done.

9) page 2, line 40, column 2: How broad is the "narrow band"? The authors should supply some estimate for the uncertainty of the scaling formula. I consider this very important.

We estimated the uncertainty of the scaling formula to 20% for the theoretical curves of the different targets, and 30% to incorporate most of the available data. The gray area drawn in Fig. 2 accounts for this uncertainty. We also included a sentence to refer to this subject in lines 119-122.

3 Reply to report of the Third Referee

This paper tries to obtain a scaling law for ionization of some biological molecules by highly charged ions. As is well known, such processes are quite relevant and important in medical physics. Since the molecules considered are complex, formal theories of ionization are difficult to apply and scaling laws, if found applicable, greatly simplify the process of obtaining reliable cross sections. In this respect the present paper is quite significant. The authors have proposed a scaling law and have applied it to several bio molecules and have tried to extend and justify the validity of the scaling law by including results for N2, O2, CO, CO2 and CH4 to show they have the same scaling behaviour. However, there are several aspects of the paper which I either do not understand clearly, or have reservations.

1. The authors mention σ to be a function of E/Z. But the functional form is nowhere mentioned in the paper. What is the functional dependence on E/Z the authors consider in the work?

In different energy regions, the ionization cross section follows different Z/E laws. At high energies, it is a function of Z^2/E, as predicted by the first Born approximation. The CDW approximation has a more complex dependence with Z/E but tends to the Born approximation at high energies, as shown in our previous work [8]. The objective of this manuscript is precisely to deepen into the study of the dependence of the ionization cross sections with Z and E in the intermediate energy region. Janev and Presnyakov [14], in their paper from 1980, suggest that σ/Z is a linear function of E/Z at intermediate energies (around the maximum of the cross sections).

In this version, we further explained the models and cross section dependence with E/Z (line 24 and the second paragraph of Section II A).

2. I have reservations in calling the scaling law developed a universal scaling law. Not only have the authors considered only 8 molecular targets and five incident ions, the results, as the authors claim, are applicable only around the maximum of the cross sections. Though this may be reasonable for practical purposes, in my opinion, the results are in too narrow range for calling it a universal scaling law. I would recommend dropping the word universal everywhere in the paper.

We called our scaling "universal" in the sense that it can be implemented for any ion-target combination within the intermediate energy range, i.e., $E/Z^{0.8} \simeq (0.04 - 5)$ MeV/amu. Nevertheless, we followed the referee's recommendation and dropped the word "universal" from the title and the rest of the manuscript. Instead, we emphasized the independent nature of the reduced scaling law for different ions and molecular targets. We also remaked that even the experimental data (in the energy range where our theoretical method starts to fail) follows the scaling proposed. In that sense, we changed the last sentence of the abstract, Section II C (lines 127-130, 136), and the Conclusions (lines 140-154, 157-160).

3. Figure 1 somehow needs to be improved or made larger, because it is very difficult to gauge the deviation of the experimental points from the curves. Is it possible to separate the figure in to two figures (eg. top four Figure 1, bottom four Figure 2)?

Separating Fig. 1 would complicate the ratio of the figure; instead, we considered convenient to make the figure larger to utilize the space better. We have also reduced the scale of the y-axis of the subplots to improve the visualization of the data.

4. Figure captions need to be significantly improved as it is difficult to read and correlate the legend descriptions with those in the figure. For the caption in Figure 2, it is not clear what the CDW-SSM theoretical results represent ? What is the target molecule considered?

We believe the confusion about Fig. 2 is originated from inconsistencies in the text. Figure 2 shows a scaling that is independent of the ion charge of the projectile and the molecular target. All the figures have the same CDW-SSM results as inputs. We improved the explanation about our calculations by adding the last paragraph of Section II B (and Eq. (2)), and the first sentence of Section II. C. The notation of Eq. (3) was slightly changed to underline that the starting point is the CDW-SSM cross sections for molecules.

Regarding points 5) and 6), we revised our manuscript and we believe it has been considerably improved.