

**Erratum: “Auger spectrum of a water molecule after single and double core ionization”  
[J. Chem. Phys. 136, 144304 (2012)]**

L. Inhester, C. F. Burmeister, G. Groenhof, and H. Grubmüller

Citation: *The Journal of Chemical Physics* **141**, 069904 (2014); doi: 10.1063/1.4892982

View online: <http://dx.doi.org/10.1063/1.4892982>

View Table of Contents: <http://scitation.aip.org/content/aip/journal/jcp/141/6?ver=pdfcov>

Published by the [AIP Publishing](#)

---

**Articles you may be interested in**

Erratum: “Core hole screening and decay rates of double core ionized first row hydrides” [J. Chem. Phys. 138, 164304 (2013)]

J. Chem. Phys. **141**, 069902 (2014); 10.1063/1.4892983

Erratum: “Spatial displacement correlations in polymeric systems” [J. Chem. Phys. 136, 164901 (2012)]

J. Chem. Phys. **139**, 029901 (2013); 10.1063/1.4813018

Erratum: “Note: Volume errors and equimolar surfaces” [J. Chem. Phys. 136, 116102 (2012)]

J. Chem. Phys. **138**, 059901 (2013); 10.1063/1.4790401

Erratum: “Beyond power laws: A new approach for analyzing single molecule photoluminescence intermittency”  
[J. Chem. Phys. 136, 184508 (2012)]

J. Chem. Phys. **137**, 099901 (2012); 10.1063/1.4748375

[Auger spectrum of a water molecule after single and double core ionization](#)

J. Chem. Phys. **136**, 144304 (2012); 10.1063/1.3700233

---



**AIP | Applied Physics  
Letters**

is pleased to announce **Reuben Collins**  
as its new Editor-in-Chief



## Erratum: “Auger spectrum of a water molecule after single and double core ionization” [J. Chem. Phys. 136, 144304 (2012)]

L. Inhester,<sup>a)</sup> C. F. Burmeister, G. Groenhof, and H. Grubmüller  
*Max Planck Institute for Biophysical Chemistry, Am Faßberg 11, 37077 Göttingen, Germany*

(Received 31 July 2014; accepted 1 August 2014; published online 13 August 2014)

[<http://dx.doi.org/10.1063/1.4892982>]

We discovered an error in our implementation of the KSG exchange potential (Eq. (12)) describing the interaction between the bound and the continuum electrons.<sup>1</sup> With the corrected implementation the values of ionization cross section and Auger decay rates slightly change without having any impact on our conclusions. The corrected Tables I–VI and Figures 3 and 5–8 calculated with correctly implemented exchange potential can be found in the supplementary material.<sup>2</sup>

<sup>1</sup>L. Inhester, C. F. Burmeister, G. Groenhof, and H. Grubmüller, “Auger spectrum of a water molecule after single and double core ionization,” *J. Chem. Phys.* **136**, 144304 (2012).

<sup>2</sup>See supplementary material at <http://dx.doi.org/10.1063/1.4892982> for Tables I–VI and Figures 3 and 5–8.

---

<sup>a)</sup>[linhest@gwdg.de](mailto:linhest@gwdg.de)