

Miron Amusia · Larissa Chernysheva
Victor Yarzhemsky

Handbook of Theoretical Atomic Physics

Data for Photon Absorption, Electron
Scattering, and Vacancies Decay



Springer

Miron Amusia
The Hebrew University
Racah Institute of Physics
Jerusalem
Israel
and
Ioffe Physica-Technical Institute
St. Petersburg
Russia

Larissa Chernysheva
Ioffe Physica-Technical Institute
St. Petersburg
Russia

Victor Yarzhemsky
Kurnakov Institute of General
and Inorganic Chemistry
Moscow
Russia

ISBN 978-3-642-24751-4 ISBN 978-3-642-24752-1 (eBook)
DOI 10.1007/978-3-642-24752-1
Springer Heidelberg New York Dordrecht London

Library of Congress Control Number: 2012940247

© Springer-Verlag Berlin Heidelberg 2012

This work is subject to copyright. All rights are reserved by the Publisher, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilms or in any other physical way, and transmission or information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed. Exempted from this legal reservation are brief excerpts in connection with reviews or scholarly analysis or material supplied specifically for the purpose of being entered and executed on a computer system, for exclusive use by the purchaser of the work. Duplication of this publication or parts thereof is permitted only under the provisions of the Copyright Law of the Publisher's location, in its current version, and permission for use must always be obtained from Springer. Permissions for use may be obtained through RightsLink at the Copyright Clearance Center. Violations are liable to prosecution under the respective Copyright Law.

The use of general descriptive names, registered names, trademarks, service marks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

While the advice and information in this book are believed to be true and accurate at the date of publication, neither the authors nor the editors nor the publisher can accept any legal responsibility for any errors or omissions that may be made. The publisher makes no warranty, express or implied, with respect to the material contained herein.

Printed on acid-free paper

Contents

Part I Photon Absorption

1	Main Points of the Theory of Photoabsorption	3
1.1	Most Important on Photoionization	3
1.2	Single Electron Hartree–Fock (HF) Approximation	5
1.3	Diagrammatical Technique	7
1.4	Many-Body Perturbation Theory	11
1.5	Random Phase Approximation with Exchange	13
1.6	Generalizations of RPAE	18
1.7	Calculation Procedures	19
1.8	Angular Anisotropy Parameter	22
1.9	Other Characteristics of Photoionization	28
1.10	Semiclosed Subshells Atoms	29
1.11	Open Shell Atoms	32
1.12	Negative and Positive Ions	34
1.13	Endohedral Atoms: The Effect of Electron Reflections	35
1.14	Endohedral Atoms: The Effect of Fullerene Polarization	39
1.15	Two-Shell Endohedrals	43
1.16	Current Induced by Photon Momentum	46
1.17	Inelastic Photoelectron Scattering	47
1.18	Satellite Excitation	49
1.19	Two-Electron Photoionization and Recombination	51
1.20	Photoionization of the Excited Atoms	54
1.21	Electron Correlations in RPAE at High Photon Energy	54
1.22	Electron Correlations at High Photon Energy Out of RPAE Frame	58
	References	59
2	Results of Calculations	65
2.1	Data Representation and Used Formulas	65
2.2	Atoms and Ions of Noble Gases	70

2.3	Atoms and Ions of Group I Elements of the Periodic Table	123
2.4	Atoms and Ions of Group II Elements of the Periodic Table	166
2.5	Ions and Atoms of Group III Elements of the Periodic Table	188
2.6	Ions and Atoms of Group IV Elements of the Periodic Table	218
2.7	Atoms and Ions of Group V Elements of the Periodic Table	232
2.8	Atoms and Ions of VI Group Elements	248
2.9	Atoms and Ions of VII and VIII Group Elements	265
2.10	Endohedral A@C ₆₀ Atoms and Ions	306
2.11	Onion-Type Endohedral Atoms A@C ₆₀ @C ₂₄₀	390
	References	414

Part II Electron Scattering

3	Main Points of the Electron Scattering Theory	421
3.1	Most Important on Electron–Atom Scattering	421
3.2	Elastic Scattering in One-Electron Approximation	427
3.3	Polarization Interaction	428
3.4	Dyson Equation	431
3.5	Inelastic Scattering of Slow and Medium Energy Electrons	432
3.6	Inelastic Scattering of Fast Particles	433
3.7	Angular Distribution of Knocked-out Electrons	438
3.8	The Compton Effect	444
3.9	GOS for Semi-filled Shells	448
3.10	Inelastic Scattering of Fast Particles upon Endohedrals	450
3.11	Bremsstrahlung of Fast Particles	456
3.12	Positron Scattering with Account of Polarization Interaction	459
	References	462
4	Electron Scattering: Results of Calculations	465
4.1	Data Representation and Used Formulas	465
4.2	Atoms of Noble Gases	467
4.3	Atoms and Some Ions of Group I Elements of the Periodic Table	574
4.4	Atoms of Group II Elements of the Periodic Table	605
4.5	Atoms and Ions of Groups IV and V Elements of the Periodic Table	639
4.6	Ions of Group VII Elements of the Periodic Table	644
4.7	Endohedral A@C ₆₀ Atoms	648
4.8	Brief Discussion of Results	669
	References	676

Part III Vacancies Decay

5	Main Points on Vacancies Decay Theory	681
5.1	Most Important About Vacancies and Their Decay	681
5.2	The Energies of Atomic Levels	684

5.3	Polarization Interaction for Vacancies	685
5.4	Self-energy Part of Green's Function and Spectroscopic Parameters	686
5.5	Satellite Lines Shapes in Photoelectron Spectra	696
5.6	Effects in Interaction Between Satellite States	699
5.7	Radiative Decay	701
5.8	Nonradiative or Auger Decay	705
5.9	Line Shapes of Low-Energy Auger Spectra	710
5.10	Two-Electron and Radiative Auger Decay	711
5.11	Single Photon Decay of Two-Hole States	714
5.12	Auger and Radiative Decay of Excited States	715
5.13	Angular Anisotropy and Spin Polarization of Auger Electrons	717
5.14	Decay of Vacancies in Endohedral Atoms	722
	References	724
6	Vacancies Decay: Results of Calculations	729
6.1	Data Presentation and Used Formulas	729
6.2	Description of Figures	730
6.3	Description of Tables	740
	References	758
7	Off-shell Photoionization Cross-sections: Results of Calculations	761
7.1	Data Presentation	761
7.2	Description of Figures	762
	References	789
8	Conclusion and Perspectives	791
	References	794
	Index	795