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Robert Thiele
PubDB Trainingskurs 2015
Hamburg, 13.10.2015



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Phys. Rev. A 86, 033411 (2012) [8 pages]

Effect of screening by external charges on the atomic orbitals and photoinduced processes within the Hartree-Fock-Slater atom

Abstract

References

Citing Articles (4)

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Robert Thiele^{1,*}, Sang-Kil Son¹, Beata Ziaja^{1,2}, and Robin Santra^{1,3}

¹Center for Free-Electron Laser Science, DESY, 22607 Hamburg, Germany

²Institute of Nuclear Physics, Polish Academy of Sciences, Radzikowskiego 152, 31-342 Kraków, Poland

³Department of Physics, University of Hamburg, 20355 Hamburg, Germany

Received 7 June 2012; published 10 September 2012

X-ray free-electron lasers (XFELs) are a promising tool for the structural determination of macro- and biomolecules, using coherent diffractive imaging. During imaging, the intense XFEL pulses also efficiently ionize the molecules, so it is important to estimate how the charged environment within the molecule modifies atomic properties, in comparison to the case of an isolated atom. Here, we apply the XATOM toolkit to obtain predictions on the modified ionization thresholds and rates of some photoinduced processes in carbon. The Hartree-Fock-Slater model is extended to include the electron screening and ion correlation effects, induced by external charges. With this extended model, we obtain predictions on modifications of orbital energies, photoabsorption cross sections, Auger decay rates, fluorescence emission rates, and atomic scattering factors as a function of the density and temperature of the surrounding charges. Our results have implications for the studies of dynamics within XFEL irradiated samples, in particular for those dedicated to coherent diffraction imaging.

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URL: <http://link.aps.org/doi/10.1103/PhysRevA.86.033411>
DOI: 10.1103/PhysRevA.86.033411
PACS: 32.80.+a, 32.80.Fb, 87.59.-e, 87.15.ag

*robert.thiele@cfel.de

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PHYSICAL REVIEW A 86, 033411 (2012)

Effect of screening by external charges on the atomic orbitals and photoinduced processes within the Hartree-Fock-Slater atom

Robert Thiele,^{1,*} Sang-Kil Son,¹ Beata Ziaja,^{1,2} and Robin Santra^{1,3}

¹Center for Free-Electron Laser Science, DESY, 22607 Hamburg, Germany

²Institute of Nuclear Physics, Polish Academy of Sciences, Radzikowskiego 152, 31-342 Kraków, Poland

³Department of Physics, University of Hamburg, 20355 Hamburg, Germany

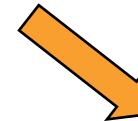
(Received 7 June 2012; published 10 September 2012)

X-ray free-electron lasers (XFELs) are a promising tool for the structural determination of macro- and biomolecules, using coherent diffractive imaging. During imaging, the intense XFEL pulses also efficiently ionize the molecules, so it is important to estimate how the charged environment within the molecule modifies atomic properties, in comparison to the case of an isolated atom. Here, we apply the XATOM toolkit to obtain predictions on the modified ionization thresholds and rates of some photoinduced processes in carbon. The Hartree-Fock-Slater model is extended to include the electron screening and ion correlation effects, induced by external charges. With this extended model, we obtain predictions on modifications of orbital energies, photoabsorption cross sections, Auger decay rates, fluorescence emission rates, and atomic scattering factors as a function of the density and temperature of the surrounding charges. Our results have implications for the studies of dynamics within XFEL irradiated samples, in particular for those dedicated to coherent diffraction imaging.

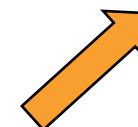
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Search for supersymmetry in hadronic final states with missing transverse energy using the variables AlphaT and b-quark multiplicity in pp collisions at 8 TeV

CMS Collaboration (Serguei Chatrchyan *et al.*) [Zeige alle 2186 Autoren](#)

Mar 12, 2013 - 43 pages

Eur.Phys.J. C73 (2013) 2568
(2013-09)
DOI: [10.1140/epjc/s10052-013-2568-6](https://doi.org/10.1140/epjc/s10052-013-2568-6)
CMS-SUS-12-028, CERN-PH-EP-2013-037
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PUBDB-2014-03626

Untersuchung des Verhaltens von Streamerkammern bei verschiedenen Gaszusammensetzungen

Poon, R. (Corresponding Author)

1995

(1995)

Report No.: PUBDB-2014-03626, WU D 95-8

Keyword(s): Unveröffentlichte Hochschulschrift

Note: Betrifft nicht POF institutional starting date
Note: Univ. of Wuppertal, Diplomarbeit, 1995

Contributing Institute(s):
1. H1 Experiment (H1(-2012))

Research Program(s):
1. Experiment HERA (H1) (POF2-511) (POF2-511)

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PUBDB-2015-02236

The Large Hadron Collider : Harvest of Run 1

Schoerner-Sadenius, T. (Editor)*

2015
Springer International Publishing Cham
ISBN: 9783319150000, 978-3-319-15000-0

Online-Ressource (2015) [10.1007/978-3-319-15001-7] LIBRARIES PDF

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Report No.: PUBDB-2015-02236

Abstract: The first run of the LHC propelled particle physics into the TeV scale, the TeV energy domain and was rewarded with the triumph of the discovery of a Higgs boson. Precision measurements of elementary cross sections and couplings so far beautifully confirmed the Standard Model, which is however known to be incomplete. Significantly increased statistics and higher energy reach may provide the sensitivity to shake its foundations, while other experiments and facilities may be needed to complete the physics interpretation.

Note: English; <http://inspirehep.net/record/1373790?ln=en>

Contributing Institute(s):

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2. Bereichsleitung FH (FH)
3. LHC/ATLAS Experiment (ATLAS)
4. International Linear Collider (ILC)
5. Theorie-Gruppe (T)

Research Program(s):

1. 611 - Fundamental Particles and their Interactions (POF3-611) (POF3-611)

Experiment(s):

1. LHC: CMS

Appears in the scientific report 2015

Linked articles:

Contribution to a book
Eisen, E. ; Grojean, C.
Perspectives on the Energy Frontier
The Large Hadron Collider : Harvests from run 1 / Schörner-Sadenius, Thomas (Editor) ; Cham : Springer International Publishing, 2015, ; ISBN: 978-3-319-15000-0 ; doi:10.1007/978-3-319-15001-7 515 - 528 (2015) [10.1007/978-3-319-15001-7] LIBRARIES PDF

Contribution to a book
Weiglein, G.
Higgs-Boson Physics at the LHC
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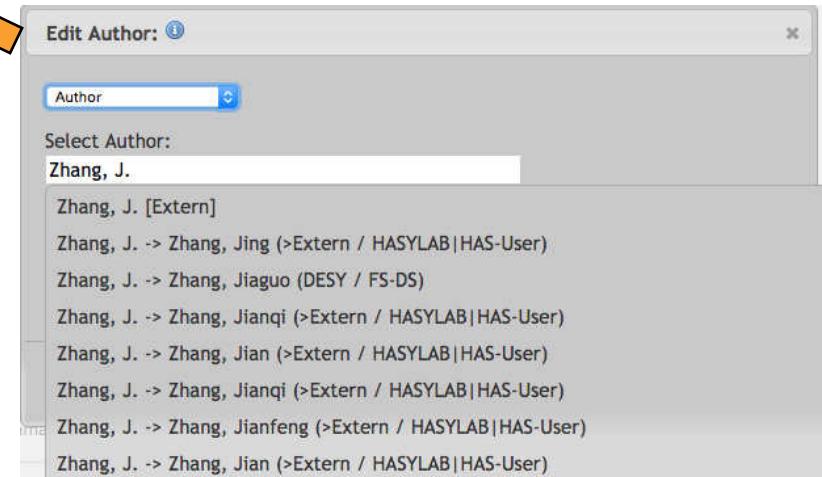
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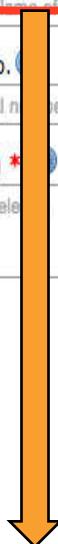
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Revision list
9 items, no notes yet last update: 14 Oct 2014, 14:15

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1. [DESY-2014-01891] Contribution to a conference proceedings/Contribution to a book
Mann, K. ; Flöter, B. ; Mey, T. ; et al/
Hartmann waveform sensor for EUV radiation
Proceedings of SPIE
Extreme Ultraviolet (EUV) Lithography IV, San Jose, California, 8679, (2013) [10.1117/12.2011508] LIBRARIES PDF

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2. [DESY-2014-01915] Contribution to a conference proceedings/Contribution to a book
Raimondi, L. ; Svetina, C. ; Mahne, N. ; et al/
K-B bendable system optimization at FERMI@Elettra FEL: impact of different spatial wavelengths on the spot size
Proceedings of SPIE: Optical Engineering + Applications
Advances in X-ray/EUV Optics and Components VIII, San Diego, California, (2013) [10.1117/12.2023024] LIBRARIES PDF

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3. [DESY-2014-03369] Contribution to a conference proceedings
Juranic, P. ; Abela, R. ; Ischebeck, R. ; et al/
THz Streak Camera for FELTemporal Diagnostics: Concepts and Considerations
36th International Free Electron Laser Conference, FEL 2014, Basel, Switzerland, 08/25/2014 - 08/29/2014 (2014)
The accurate, non-destructive measurements of FEL pulse length and arrival time relative to an experimental laser are necessary for operators and users alike. The FEL operators can get a better understanding of their machine and the optics of an FEL by examining the pulse length changes of the photons coming to the user stations, and the users can use the arrival time and pulse length information to better understand their data. [...]
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4. [DESY-2014-03784] Journal Article
Feneberg, M. ; Osterburg, S. ; Romero, M. F. ; et al/
Optical properties of magnesium doped Al_xGa_{1-x}N (0.61 ≤ x ≤ 0.73)
Journal of applied physics 116(14), 143103 - (2014) [10.1063/1.4897449] PDF

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5. [DESY-2014-03782] Contribution to a book
Stana, M. ; Ross, M. ; Sepiol, B.
Atomic Migration Studies with X-Ray Photon Correlation Spectroscopy
Diffusion Foundations 2, (2014) [10.4028/www.scientific.net/DF.2.73] LIBRARIES PDF
The new technique of atomic-scale X-ray Photon Correlation Spectroscopy (aXPCS) makes use of a coherent X-ray beam to study the dynamics of various processes in condensed matter systems. Particularly atomistic migration mechanisms are still far from being understood in most of intermetallic alloys and in amorphous systems. Special emphasis must be given to the opportunity to measure atomistic diffusion at relatively low temperatures where such measurements were far out of reach with previously established methods. [...]

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6. [PUBDB-2014-03434] Review/Contribution to a book
Fischer, G. ; Selvadurai, U. ; Nellesen, J. ; et al/
Analysis of stress gradients in physical vapour deposition multilayers by X-ray diffraction at fixed depth intervals
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Journal Article PHPPUBDB-14596

Thomson scattering on inhomogeneous targets

Thiele, R. *; Sperling, P.; Chen, M. W.; Bornath, T.; Faeustlin, R. R.; Fortmann, C.; Glenzer, S. H.; Kraeft, W.-D.; Pukhov, A.; Toleikis, S. *; Tschentscher, T. *; Redmer, R.

2010
APS College Park, Md.

Physical review / E 82, 056404 (2010) [10.1103/PhysRevE.82.056404] LIBRARIES PDF >>

Please use doi:10.1103/PhysRevE.82.056404 in citations.

Report No.: PHPPUBDB-14596

Contributing Institute(s):

1. European XFEL (XFEL(-2012))
2. Experiments with synchrotron radiation (HASYLAB(-2012))

Research Program(s):

1. FLASH Beamline BL2 (POF2-54G16) (POF2-54G16)

Experiment(s):

Appears in the scientific report 2010

Database coverage:
JCR

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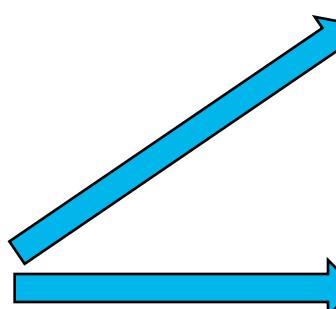
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Group(s) directly involved * ⓘ

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MPY: Beschleunigerphysik

FS-US: FS-Undulator Systeme

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Author(s) / Contributer(s) / Editor(s) * ⓘ

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Keil, Joachim -> Keil, Joachim (DESY / MPY) Author

Kling, A. [Extern] Author

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Distributions of topological observables in inclusive three- and four-jet events in pp collisions at $\sqrt{s} = 7$ TeV
[CMS-QCD-11-006; CERN-PH-EP-2014-302; arXiv:1502.04785]
The European physical journal / C 75(7), 302 (2015) [10.1140/epjc/s10052-015-3491-9] This paper presents distributions of topological observables in inclusive three- and four-jet events produced in pp collisions at a centre-of-mass energy of 7 TeV with a data sample collected by the CMS experiment corresponding to a luminosity of 5.1 fb^{-1} . The distributions are corrected for detector effects, and compared with several event generators based on two- and multi-parton matrix elements at leading order. [...]
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Talk (non-conference) PUBDB-2015-03875

PubDB-Training 2015

Thiele, R. (Corresponding author)*

2015

(2015)

Report No.: PUBDB-2015-03875

Abstract: Dieses Jahr liegt der Fokus bei der POF3, verknüpfte Records und Volltexte (Open Access), sowie bei den wichtigen Neuerungen im System.

Editorenenschulung, Hamburg, DESY, Germany, 13 Oct 2015

Contributing Institute(s):

- Bibliothek und Dokumentation (L)

Research Program(s):

- 899 - ohne Topic (POF3-899) (POF3-899)
- JOIN² - Just anOther INvenio INstance (JOIN2-2014) (JOIN2-2014)

Experiment(s):

- No specific instrument

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