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Robert Thiele

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Hamburg, 4.12.2013

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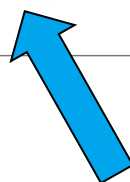
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APS » Journals » Phys. Rev. A » Volume 86 » Issue 3

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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

10.1103/PhysRevA.86.033411

*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

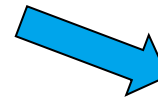
(Received 7 June 2012; published 10 September 2012)

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.

DOI: 10.1103/PhysRevA.86.033411

PACS number(s): 32.90.+a, 32.80.Fb, 87.59.-e, 87.15.ag

10.1103/PhysRevA.86.033411



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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](#)
CMS-SUS-12-028, CERN-PH-EP-2013-037
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DESY-2013-01221

Herwig++ 2.7 Release Note

Bellm, J. ; Gieseke, S. ; Grellscheid, D. ; Papaefstathiou, A. ; Platzer, S. ; Richardson, P. ; Rohr, C. ; Schuh, T. ; Seymour, M. H. ; Siodmok, A. ; Wilcock, A. ; Zimmermann, B.

2013

(2013)

Report No.: DESY-2013-01221, DESY 13-186

Abstract: A new release of the Monte Carlo event generator Herwig++ (version 2.7) is now available. This version comes with a number of improvements including: an interface to the Universal FeynRules Output (UFO) format allowing the simulation of a wide range of new-physics models; developments of the Matchbox framework for next-to-leading order (NLO) simulations; better treatment of QCD radiation in heavy particle decays in new-physics models; a new tune of underlying event and colour connection parameters that allows a good simultaneous description of both Tevatron and LHC underlying event data and the effective cross-section parameter for double-parton scattering.

Note: erwig++, arXiv:1310.6877

Contributing Institute(s):

1. Theorie-Gruppe (T)

Research Program(s):

1. 514 - Theoretical Particle Physics (POF2-514)

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Report Number ⓘ
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Thiele, Robert -> Thiele, Robert (>DESY / L) Corresponding author	✓	✕
Son, Sang-Kil -> Son, Sang-Kil (>DESY, >CFEL / FS-CFEL-3) Author	✓	✕
Ziaja, Beata -> Ziaja-Motyka, Beata (>DESY, >CFEL / FS-CFEL-3) Author	✓	✕
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Title * ⓘ
Effect of screening by external charges on the atomic orbitals and photoinduced processes within

Journal * ⓘ Physical review / A

DOI ⓘ 10.1103/PhysRevA.86.03

Volume * ⓘ 86 Issue ⓘ 3 Pages * ⓘ 033411

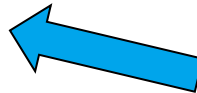
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Ziaja, Beata ->
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Santra, Robin
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Institution:
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>CFEL: Centre for Free-Electron Laser Science
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ATLAS, CFEL, MKK1,...

FS-BT: FS-Beamline Technology

FS-DO: FS-Experimentenbetreuung DORIS

FS-DS: FS-Detektor Systeme

FS-EC: FS-Experiment Control

FS-FL: Experimentenbetreuung FLASH

FS-ML: FS-Arbeitsgruppe

FS-NL: Nanolab

FS-PE: Experimentenbetreuung PETRA III

FS-PEX: PETRA III Extension

FS-TI: FS-Arbeitsgruppe

FS-US: FS-Undulator Systeme

Largescale Facility/Beamline * ⓘ

DORIS Beamline A1

DORIS Beamline A2

DORIS Beamline B1

DORIS Beamline B2

DORIS Beamline BW1

DORIS Beamline BW2

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DORIS Beamline BW6

DORIS Beamline BW7

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mueller, (Extern) Corresponding author

mueller, -> Mueller, Katharina (>Extern, >Extern / H1/ZUER) Corresponding author

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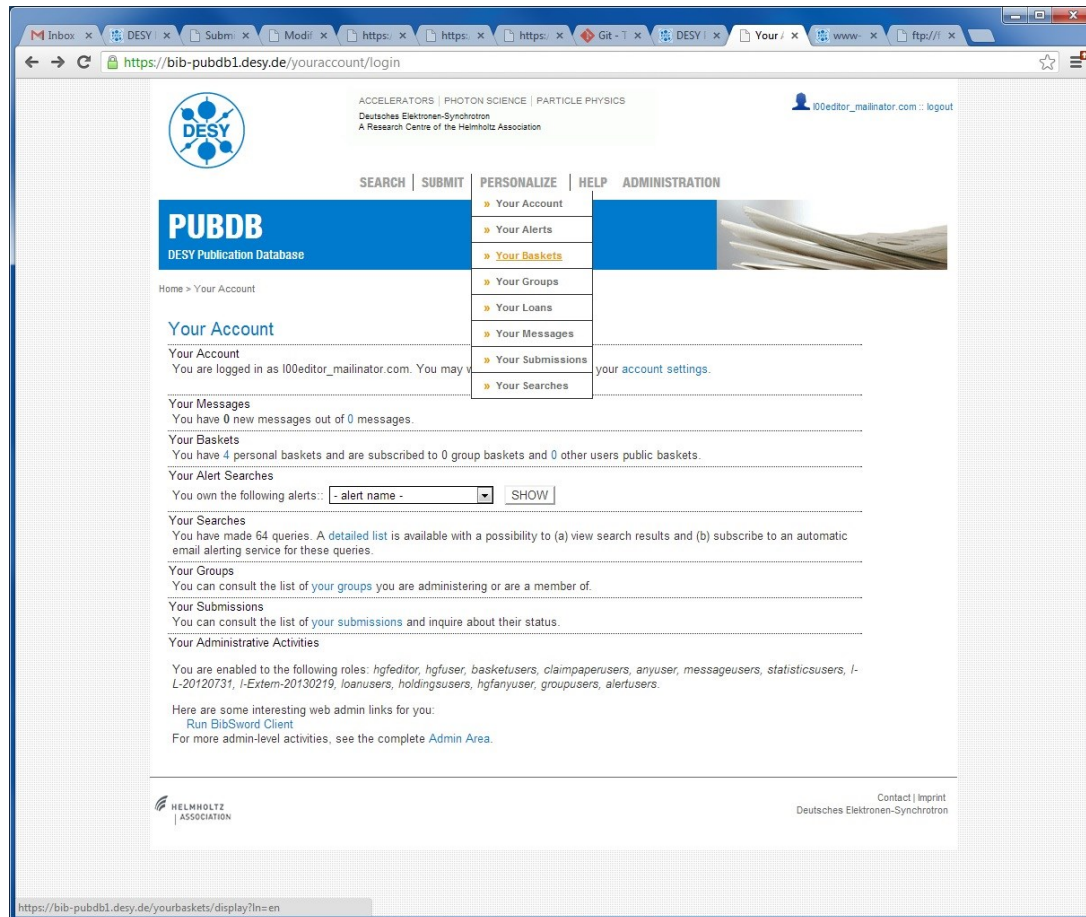
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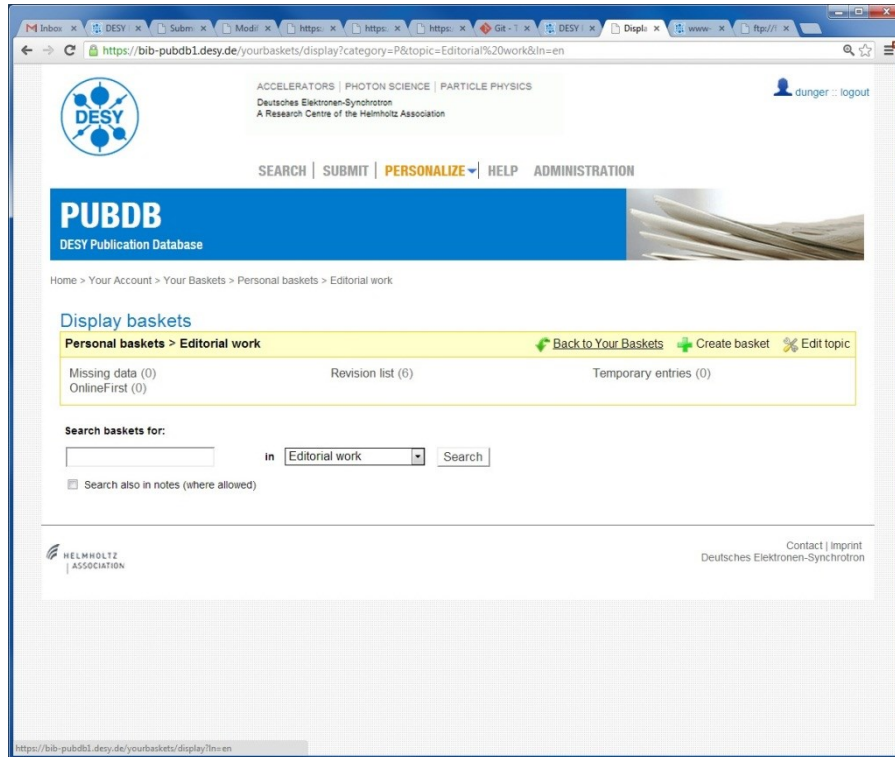


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Revision list

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last update: 06 Jun 2013, 16:30

1. [DESY-2013-00109] Conference Presentation (Panel discussion)
Zozulya, A.; Bartsch, T.; Heyn, C.; et al
Coherent x-ray diffraction study of GaAs nanopillars embedded in air-gap heterostructures
E-MRS 2013 SPRING MEETING, E-MRS 2013, Strassbourg, France, 05/27/2013 - 05/31/2013 (2013)
Recent advances in nanofabrication reveal significant impact of nanostructuring on thermal transport in solids. This paves a way for thermoelectric devices with low thermal conductance. [...]
External link: http://www.emrs-strasbourg.com/index.php?option=com_abstract&task=view&id=198&day=2013-05-29&year=2013&Itemid=99999999&id_season=9
Detailed record - Add a note... Copy item Remove item

2. [DESY-2013-00112] Journal Article
Mozzanica, A.; Bergamaschi, A.; Dinapoli, R.; et al
The GOTTHARD charge integrating readout detector: design and characterization
Journal of Instrumentation 7(01), C01019 - C01019 (2012) [10.1088/1748-0221/7/01/C01019]
Detailed record - Add a note... Copy item Remove item

3. [DESY-2013-00115] Dissertation / PhD Thesis/Internal Report
Zhang, J.
X-ray Radiation Damage Studies and Design of a Silicon Pixel Sensor for Science at the XFEL
[DESY-THESIS-2013-018]
(2013)
Experiments at the European X-ray Free Electron Laser (XFEL) require silicon pixel sensors which can withstand X-ray doses up to 1 GGy. For the investigation of X-ray radiation damage up to these high doses, MOS capacitors and gate-controlled diodes built on high resistivity n-doped silicon with crystal orientations <100> and <111> produced by four vendors, CIS, Hamamatsu, Canberra and Sinfel, have been irradiated with 12 keV X-rays at the DESY DORIS III synchrotron-light source. [...]
Fulltext: PDF
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4. [DESY-2013-00114] Journal Article
Asmara, T. C.; Wang, X.; Santoso, I.; et al
Large spectral weight transfer in optical conductivity of SrTiO₃ induced by intrinsic vacancies
Journal of physics / Condensed matter 0, 1-5 (2012)
The optical conductivity (σ_{imag}) of SrTiO₃ for various vacancies has been systematically studied using a combination of ultraviolet - vacuum ultraviolet (UV-VUV) reflectivity and spectroscopic ellipsometry. For cation (Ti) vacancies, σ_{imag} shows large spectral weight transfer over a wide range of energy from as high as 35 eV to as low as 0.5 eV and the presence of mid-gap states, suggesting that strong correlations play an important role. [...]
Fulltext: PDF
External link: <http://arxiv.org/abs/1206.6686v2>
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5. [DESY-2013-00108] Journal Article
Gutt, C.; Streit-Nierobisch, S.; Walther, M.; et al
Endstation for ultrafast magnetic scattering experiments at the free-electron laser in Hamburg
Review of scientific instruments 84(1), 013906 - (2013) [10.1063/1.4773543]

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Journal Article (0) PHPPUBDB-14596

Thomson scattering on inhomogeneous targets

Thiele, R. ; Sperling, P. ; Chen, M. ; Bornath, T. ; Fäustlin, 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] 

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

Report No.: PHPPUBDB-14596

Contributing Institute(s):

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

Research Program(s):

1. FLASH Beamline BL2 (POF2-54G16)

Appears in the scientific report 2010

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