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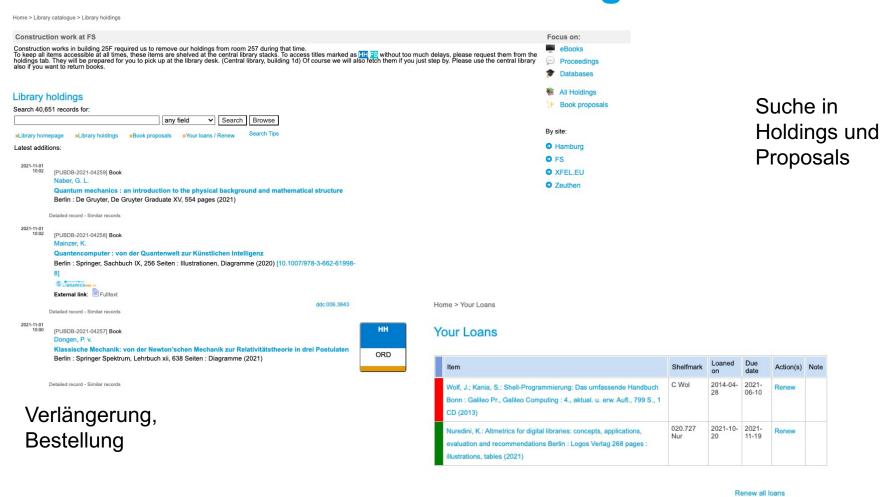
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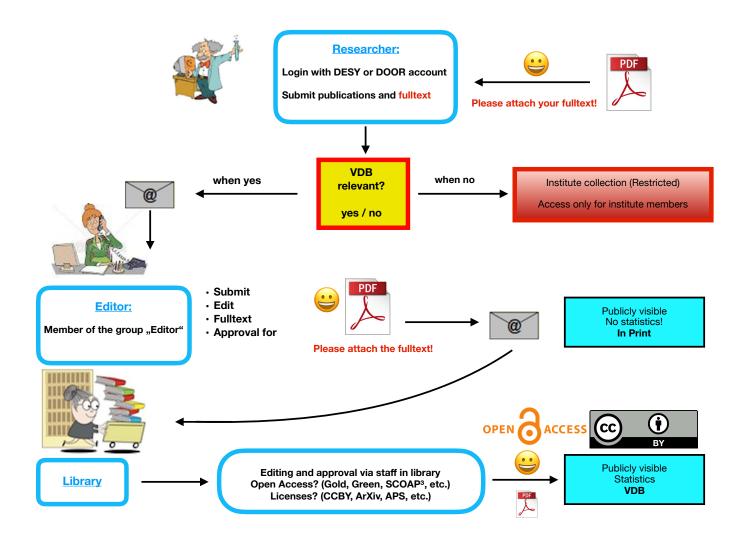


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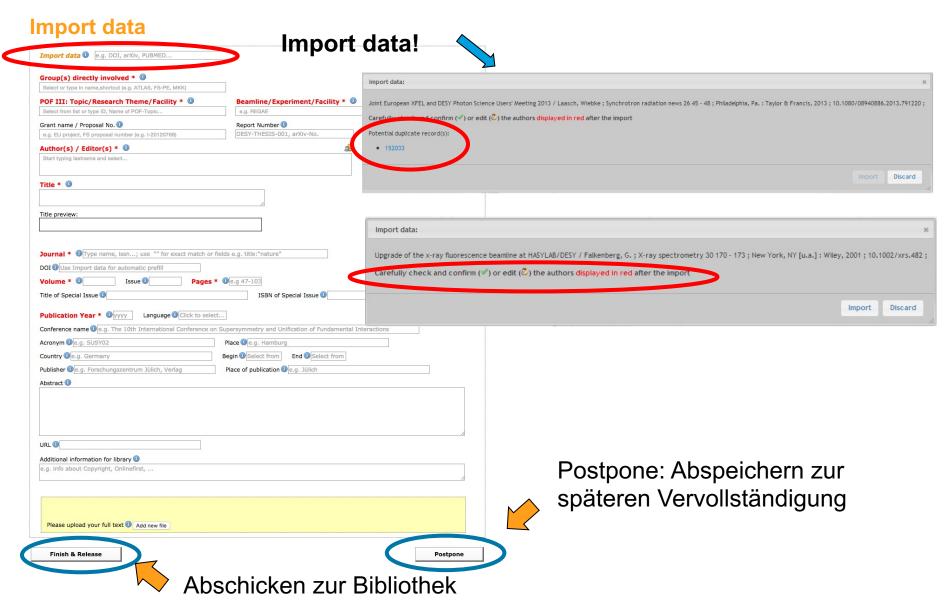
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Effect of screening by external charges on the atomic orbitals and photoinduced processes within the Hartree-Fock-Slater atom

Citing Articles (4) Download: PDF (559 kB) Export: BibTeX or EndNote (RIS)

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

References

Center 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

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OKL: http://link.aps.org/doi/10.1103/ DOI: 10.1103/PhysRevA.86.033411

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Abstract

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10.1103/PhysRevA.86.033411





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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

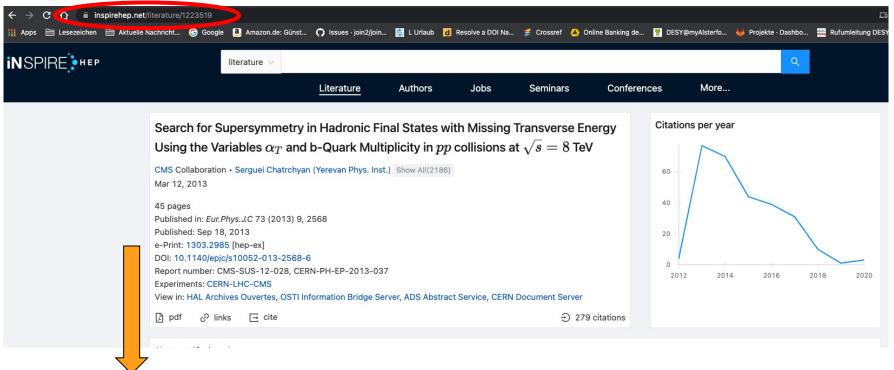
Robert Thiele, 1,* Sang-Kil Son, 1 Beata Ziaja, 1,2 and Robin Santra 1,3 ¹Center for Free-Electron Laser Science, DESY, 22607 Hamburg, Germany ²Institute of Nuclear Physics, Polish Academy of Sciences, Radzikowskiego 152, 31-342 Kraków, Poland ³Department of Physics, University of Hamburg, 20355 Hamburg, 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

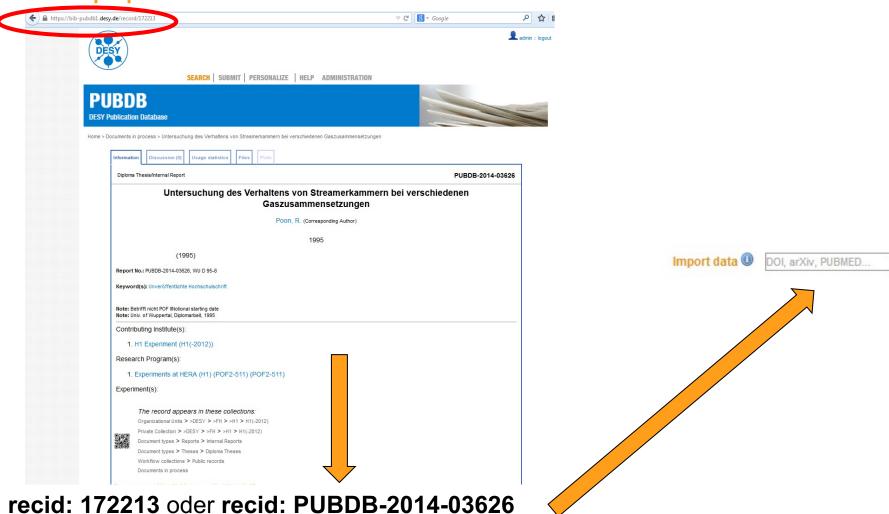
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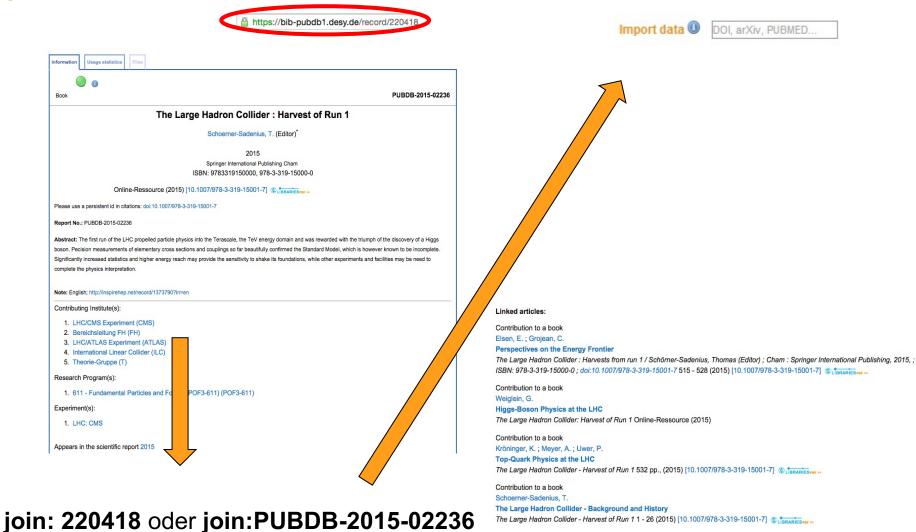


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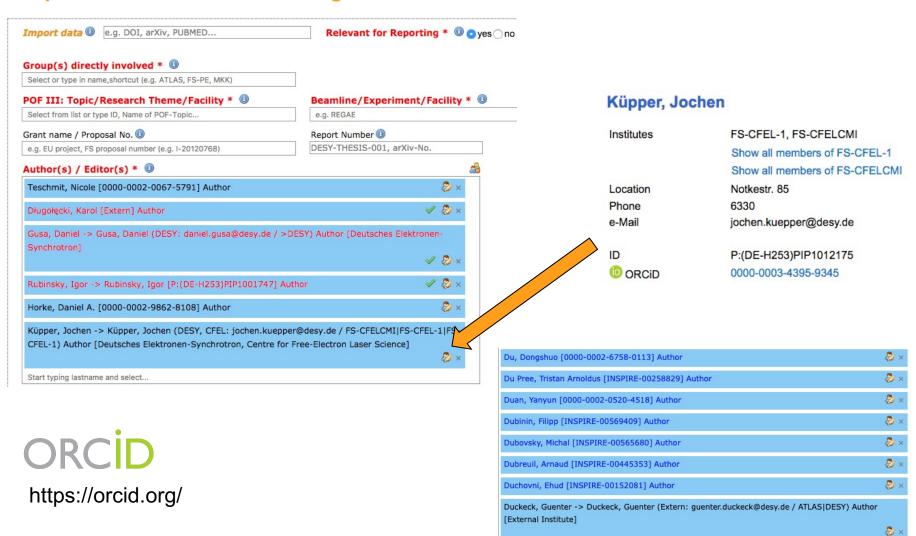
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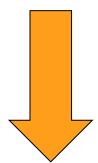
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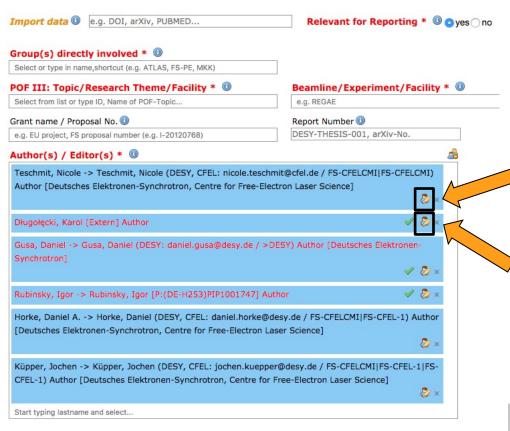
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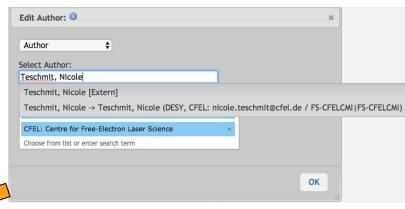
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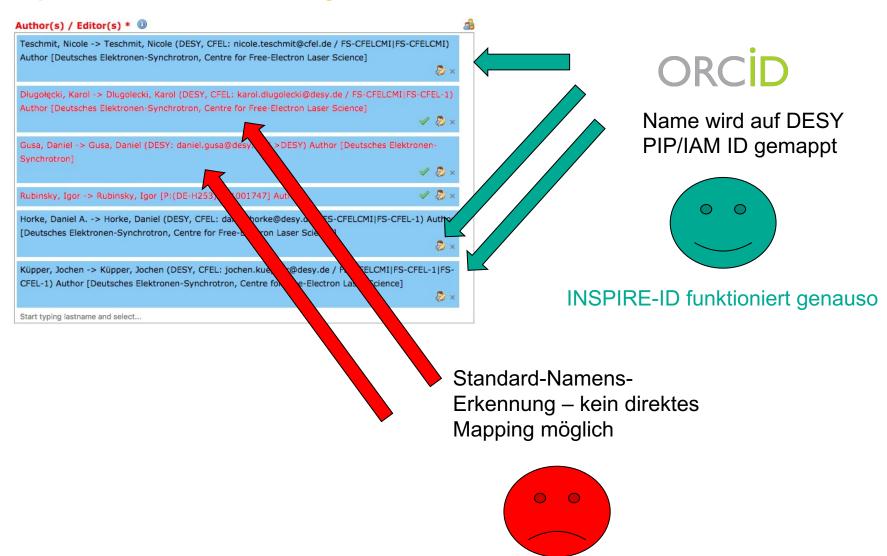
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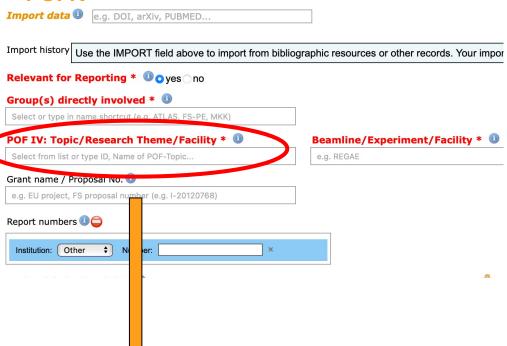
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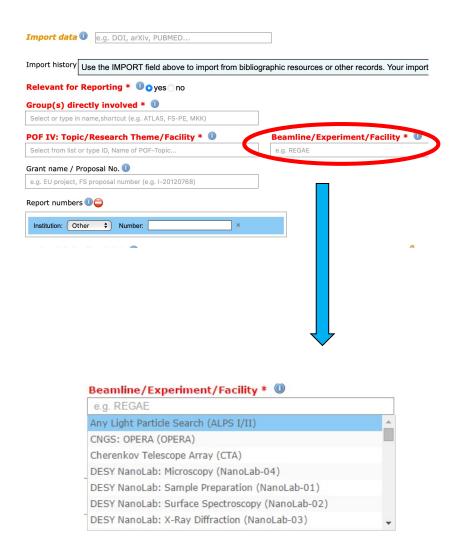
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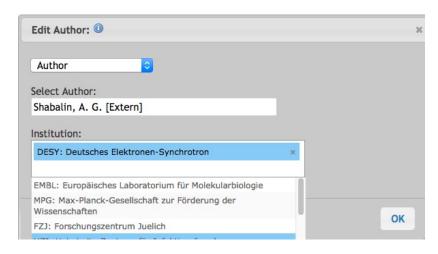
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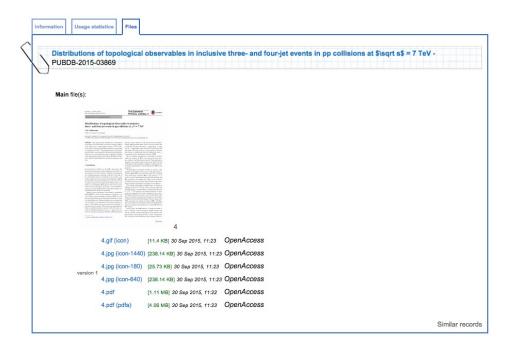
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[CMS-QCD-11-006; CERN-PH-EP-2014-302; arXiv:1502.04785]

The European physical journal / C 75(7), 302 (2015) [10.1140/epjc/s10052-015-3491-9]

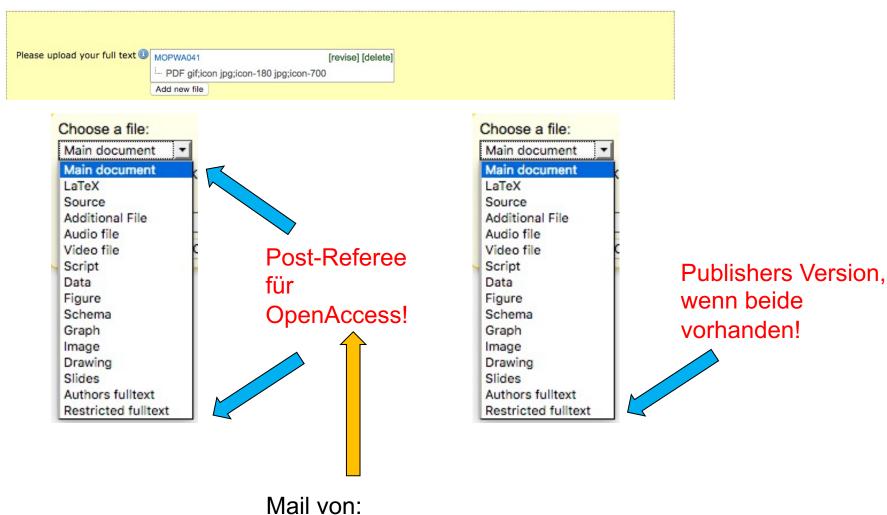
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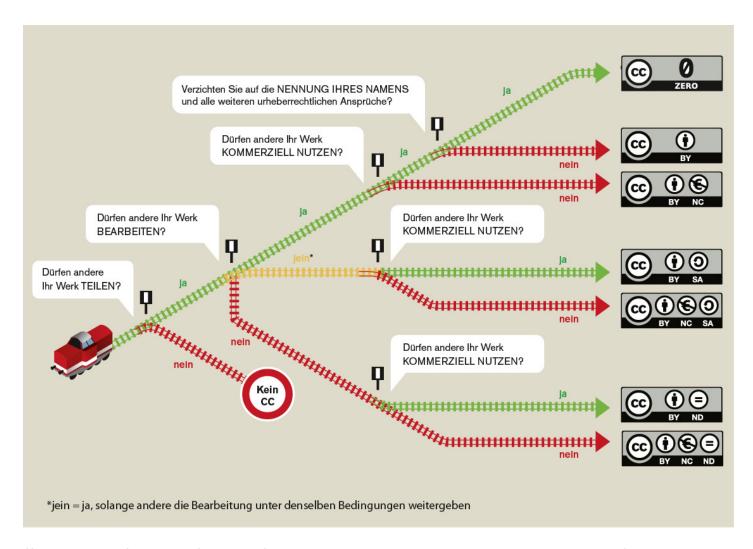
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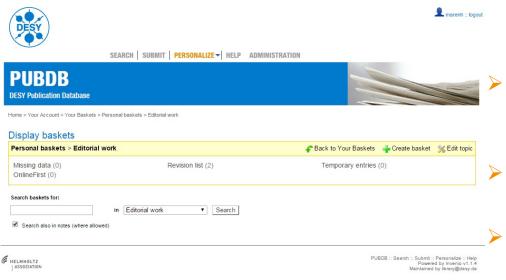
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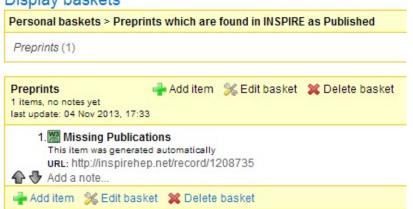
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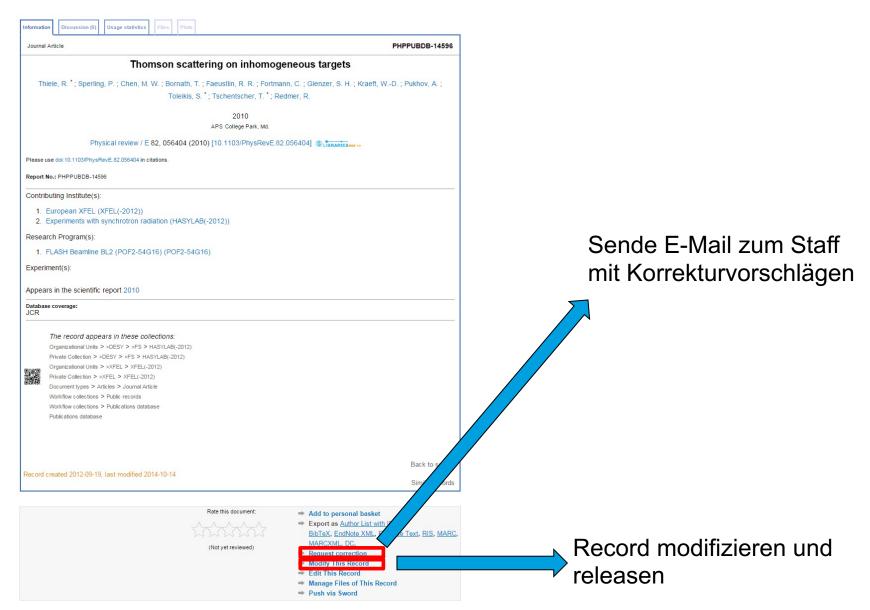
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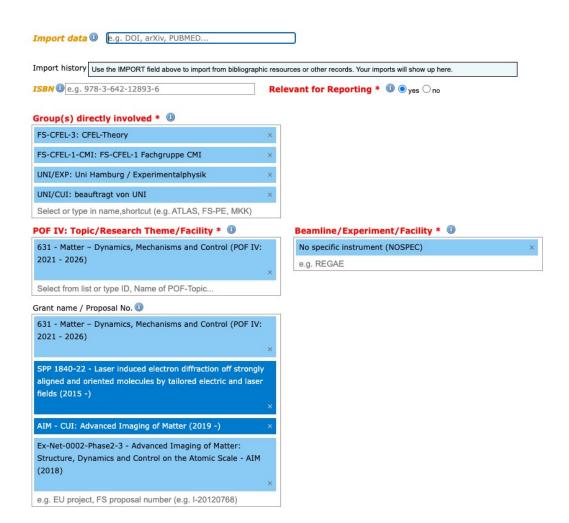


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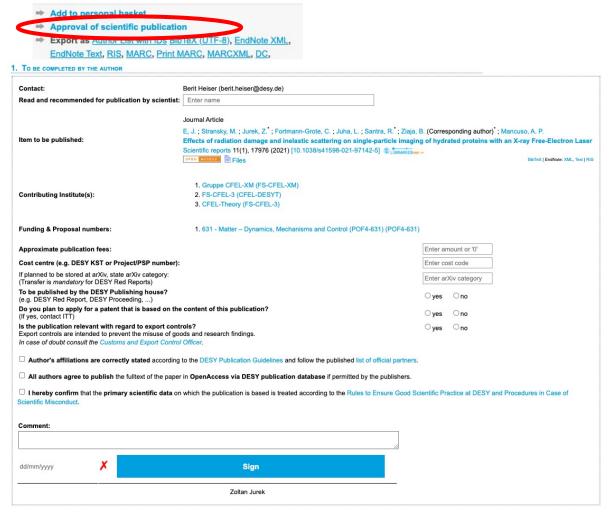


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High intensity x-ray interaction with a model bio-molecule system: double-core-hole states and fragmentation of formamide

Journal of physics / B 53(24), 244005 (2020) [10.1088/1361-6455/abc183] Files Fulltext





Karamatskos, E.; Yarlagadda, S.; Patchkovskii, S.; Vrakking, M.; Welsch, R.; Küpper, J. (Corresponding author); Rouzée, A. (Corresponding author) Time-resolving the UV-initiated photodissociation dynamics of OCS Faraday discussions 228, 413 - 431 (2020) [10.1039/D0FD00119H] Files BibTeX | EndNote: XML, Text | RIS



Wang, J. (First author); Kilaj, A.; He, L.; Długołęcki, K.; Willitsch, S. (Corresponding author); Küpper, J. (Corresponding author)

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The journal of physical chemistry <Washington, DC> / A 124(40), 8341-8345 (2020)

[10.1021/acs.jpca.0c05893] special issue: "Daniel Neumark Festschrift" B OPEN ACCESS Files Fulltext BibTeX | EndNote: XML, Text | RIS



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Kilaj, A.; Gao, H.; Tahchieva, D. N.; Ramakrishnan, R.; Bachmann, D. G.; Gillingham, D.; von Lilienfeld, A.; Küpper, J.; Willitsch, S. (Corresponding author)

Quantum-chemistry-aided identification, synthesis and experimental validation of model systems for conformationally controlled reaction studies: Separation of the conformers of 2,3-dibromobuta-1,3-diene in the gas phase

Physical chemistry, chemical physics 22(24), 13431 - 13439 (2020) [10.1039/D0CP01396J]

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 Nanoclusters from Combined Pair Distribution Function and Small-Angle X-ray
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[10.1002/anie.202103641] ($\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\exitit{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\exitit{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\exitit{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\}\exitit{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\tex{$\text{$\text{$\text{$\text{$\}}}}\text{$\text{$\text{$\text{$\}\exitit{$\text{$\text{$\text{$\text{$\text{$\text{$\text{$\text{
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 Šmilauerová, J.; Doležal, P.; Veselý, J.; Semenova, I.; Polyakova, V.; Janeček, M.
In-situ investigation of phase transformations in ultra-fine grained Ti15Mo alloy
 Journal of alloys and compounds 867, 159027 (2021) [10.1016/j.jallcom.2021.159027]
 LIBRARIES POF >>
  Fulltext
                                                                                                                      BibTeX | EndNote: XML, Text | RIS
```

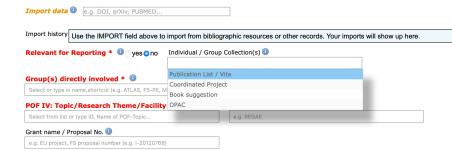
PubDB – Literaturlisten in Webseiten.



- Bedienung der Webseiten direkt aus der PubDB
- Aussehen in Abhängigkeit des auf der Webseite benutzten Style
- Import von Queries (Bibliothek bietet Hilfe dafür an) durch das Invenio-Plugin im ZMS / CMS
- Queries via verbesserten Search Generator

Vorteile:

- Neue Publikationen nach PubDB-Submit automatisch
- Outputformat gsblst: Nature
- Links zu Titel, Autoren: höheres Google-Ranking
- Bessere Sichtbarkeit und professionelle
 Darstellung eigener
 Arbeiten
- Weniger Arbeit dank DOI-Import / INSPIRE-Import und Nutzung normierter Datensätze
- Wichtig: Auch VITA-Publikationen möglich!



PubDB - Statistiken.

Link direkt auf der Startseite!

HGFStatistics - Parameters for calculation

Please fill out with year or year range: 2017 or 2010->2017

At least one internal author? yes

At least one external author? no 💌

POF Period: POF III

Calculation of: ✓ POF ✓ Institutes □ Grants □ Experiments □ Conferences

Please note: If more selected, the calculation time increases significantly!

Last / First author (DKFZ only) no

Additional Parameters:

Collection: VDB

WEB year: yes •

Cache: yes •

Calculate

Quick Links Search Generator Statistics Formular POF Overview Exp/BL Overview Inst/Group Overview Library Home ORCID

Show 10 entries					Search:		
A	2015 🖣	2016 🖣	2017 🖣	2018	2019	2020 🖣	2021 🖣
600 - Forschungsbereich Materie (POF III: 2015 - 2020)	833	940	903	1001	993	1098	0
600 - Forschungsbereich Materie (POF IV: 2021 - 2026)	0	0	0	0	0	3	541
610 - Materie und Universum (POF III: 2015 - 2020)	434	541	488	551	520	546	0
610 - Matter and the Universe (POF IV: 2021 - 2026)	0	0	0	0	0	2	242
611 - Fundamental Particles and Forces (POF III: 2015 - 2020)	355	443	392	457	412	409	0
611 - Fundamental Particles and Forces (POF IV: 2021 - 2026)	0	0	0	0	0	2	201

OpenAccess Rates (WOS/Scopus) in Percent

108

137

0

Direkte Open Access Quoten in Tabellen für POF,

613 - Matter and Radiation from the Universe (POF III: 2015 - 2020)

613 - Matter and Radiation from the Universe (POF IV: 2021 - 2026)

620 - Matter and Technologies (POF IV: 2021 - 2026)

620 - Von Materie zu Materialien und Leben (POF III: 2015 - 2020)

Showing 1 to 10 of 39 entries

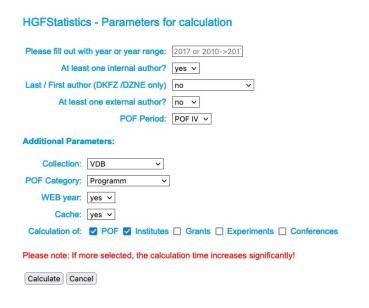
Gruppen und Experimente

Show 10 S entries Search:												
	^ 20	15 🔷	2016 🖣	2017 👇	2018 🖣	2019 🖣	2020 🖣	2021 👇				
600 - Forschungsbereich Materie (POF III: 2015 - 2020)	81%		86%	86%	91%	90%	81%	-				
600 - Forschungsbereich Materie (POF IV: 2021 - 2026)	-		-	-	-	-	67%	87%				
610 - Materie und Universum (POF III: 2015 - 2020)	97%		100%	98%	99%	98%	89%	-				
610 - Matter and the Universe (POF IV: 2021 - 2026)	-		-	-	-	-	50%	90%				
611 - Fundamental Particles and Forces (POF III: 2015 - 2020)	98%		100%	99%	99%	99%	94%	-				
611 - Fundamental Particles and Forces (POF IV: 2021 - 2026)	-		-	-	-	-	50%	97%				
613 - Matter and Radiation from the Universe (POF III: 2015 - 2020)	92%		98%	95%	98%	91%	74%	-				
613 - Matter and Radiation from the Universe (POF IV: 2021 - 2026)	-		-	-	-	-	-	56%				
620 - Matter and Technologies (POF IV: 2021 - 2026)	-		-	-	-	-	-	85%				
620 - Von Materie zu Materialien und Leben (POF III: 2015 - 2020)	61%		67%	71%	82%	82%	72%	-				
Showing 1 to 10 of 39 entries					Draviou	. 1	2 2	A Nove				

Showing 1 to 10 of 39 entries

PubDB - Statistiken.

Mögliche Parameter



Wofür das Ganze?:

- Einfacher und schneller Überblick für die Gruppen: Ist alles drin?
- POF Berichterstattung: Was wurde oder wird gezählt?
- Qualitätssicherung und Management
- Erstellung von Literaturlisten

- Welches Jahr, welcher Zeitraum?
- Ist mindestens ein interner Autor dabei?
- Ist mindestens ein externer Autor dabei?
- Auswahl der POF-Periode (POF I-IV) ab November Release
- Collection (Veröffenlichungsdatenbank, Vita oder Open Access)
- Welche Kategorie? (Forschungsbereich, Programm, Topic, Subtopic)
- Rechnung für wissenschaftlichen Ergebnisbericht?
- Welche Teile will man berechnen?

PubDB - Statistiken.

Automatisierte Tabellen für POF und Gruppen

Per institute and statistics key

Show 10 ont	how 10 o entries													ch: Theory							
A	WOS + Scopus (POFIII / POFIV Indikator)	WOS listed journal OR entry (POFII Indikator)	All of WoS and Scopus listed	Scopus listed	Thomson Reuters Master Journal List	JCR listed	WOS and not JCR	Web of Science	Other refereed	User supplied Peer Review	Refereed NOT in WoS	Refereed but NOT in WOS or Scopus	All refereed	Pubmed listed	DOAJ listed	TRMJL but no	TRMJL: 0< IF <5	TRMJL: 5<= IF <10			
Theory	83	82	83	81	80	78	0	80	82	0	10	10	93	40	55	2	28	50			
Theory-HH	67	66	67	65	65	63	0	65	66	0	9	9	76	27	47	2	17	46			
Theory- Zeuthen	16	16	16	16	15	15	0	15	16	0	1	1	17	13	8	0	11	4			

Showing 1 to 3 of 3 entries (filtered from 51 total entries)

Showing 1 to 3 of 3 entries (filtered from 51 total entries)

Per institute and document type

Search: Theory														
Dissertation / PhD Thesis	Internal Report	Journal Article	Lecture +	Master Thesis	Bachelor Thesis	Poster +	Preprint +	Proceedings -	Report 🖣	Book 🖣	Talk (non- conference)	Conference Presentation	Contribution to a book	Contribution to a conference proceedings
4	0	93	4	1	0	0	87	0	179	4	37	47	0	8
4	0	76	4	1	0	0	75	0	155	4	37	47	0	7
0	0	17	0	0	0	0	12	0	24	0	0	0	0	1
	Dissertation / PhD Thesis	Dissertation / PhD Thesis Internal Report 4 0 4 0	Dissertation / PhD Thesis Internal Report Article 4 0 93 4 0 76	Dissertation	Dissertation	Dissertation	Dissertation	Dissertation / PhD Thesis Internal Report Journal Article Lecture Master Thesis Bachelor Thesis Poster Preprint 4 0 93 4 1 0 0 87 4 0 76 4 1 0 0 75	Dissertation / PhD Thesis Internal Report Journal Article Lecture Master Thesis Bachelor Thesis Poster Preprint Proceedings 4 0 93 4 1 0 0 87 0 4 0 76 4 1 0 0 75 0	Dissertation / PhD Thesis Internal Report Journal Article Lecture Master Thesis Bachelor Thesis Poster Preprint Proceedings Report 4 0 93 4 1 0 0 87 0 179 4 0 76 4 1 0 0 75 0 155	Dissertation	Dissertation / PhD Thesis Internal Report Journal Article Lecture Master Thesis Poster Thesis Preprint Proceedings Report Book Talk (non-conference) 4 0 93 4 1 0 0 87 0 179 4 37 4 0 76 4 1 0 0 75 0 155 4 37	Dissertation / PhD Thesis Internal Report Journal Article Lecture Master Thesis Poster Thesis Preprint Proceedings Report Book Talk (non-conference) Conference Presentation 4 0 93 4 1 0 0 87 0 179 4 37 47 4 0 76 4 1 0 0 75 0 155 4 37 47	Dissertation / PhD Thesis Internal Report Journal Article Lecture Master Thesis Poster Thesis Preprint Proceedings Report Book Talk (non-conference) Conference Presentation Contribution to a book 4 0 93 4 1 0 0 87 0 179 4 37 47 0 4 0 76 4 1 0 0 75 0 155 4 37 47 0

Überblick der POF-Programme, Gruppen, Grants, Experimente oder Konferenzen:

- Aufschlüsselung aller relevanter Publikationstypen / statistischen Schlüssel
- Komplett als Hyperlinks zu den Suchabfragen aufgebaut
- Voll durchsuchbar und individuell einstellbar

Ausblick.



- POFIV wurde 2021 implementiert, Erstellung der Normdatensätze, Erfassung von Altdaten
- Anbindung der Personendatensätze an das IAM (UTF8, ORCID, aktuell)
- Betrieb mit Docker um das Ausrollen der monatlichen Releases zu vereinfachen
- Wir arbeiten an neuen Submit-Masken für ein mögliches Nachfolgesystem



https://bib-pubdb1.desy.de/record/470848