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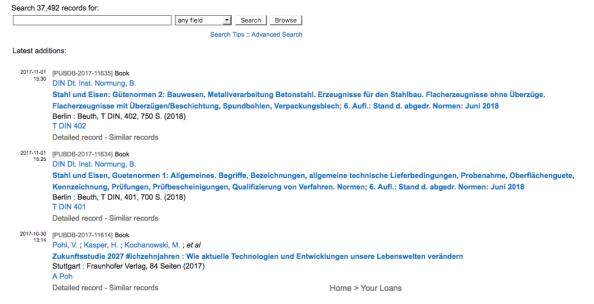
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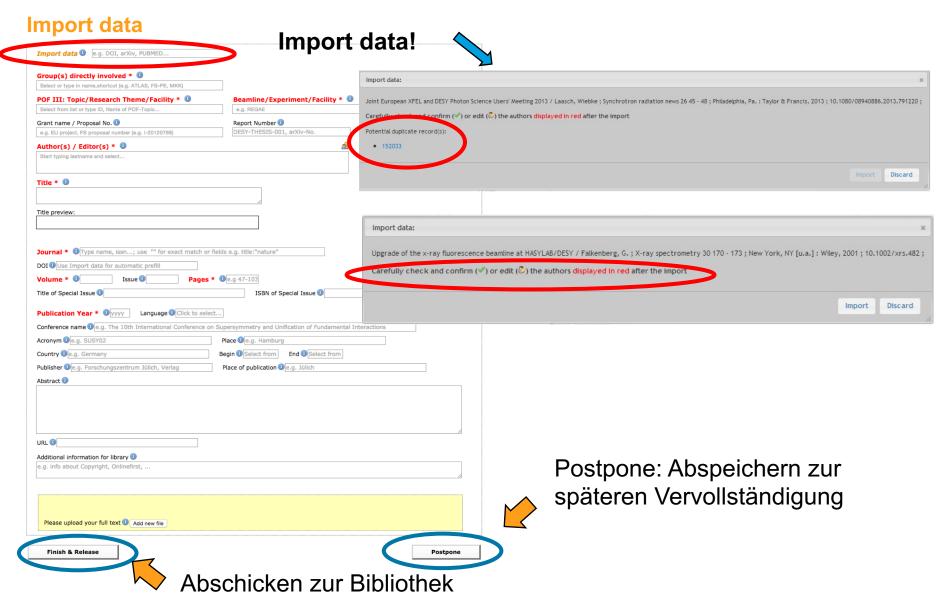
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Phys. Rev. A 86, 033411 (2012) [8 pages]

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

Citing Articles (4)

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

References

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 XMTOM 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/Pnysit. 1.96.033 DOI: 10.1103/PhysRevA.86.033411

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Abstract

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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}

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

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

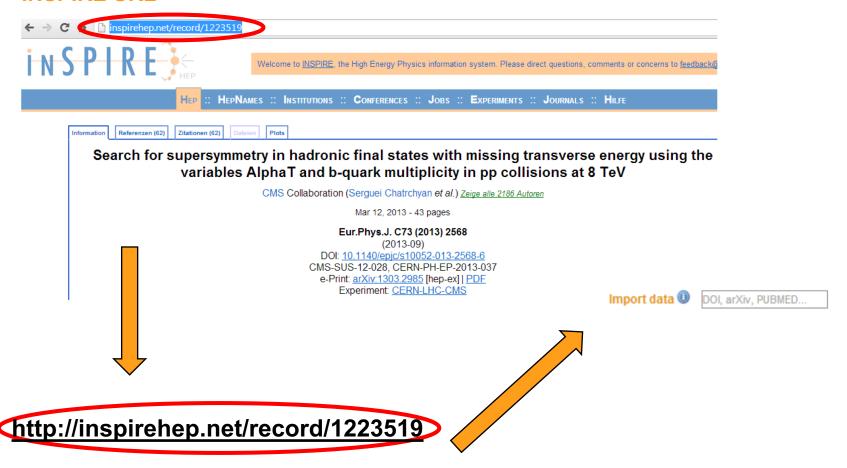
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X-ray free-electron lasers (XFELs) are a promising tool for the structural determination of macro- and biomolecules, using coherent diffractive imaging. During imaging, the intense XFEL pulses also efficiently ionize the molecules, so it is important 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.

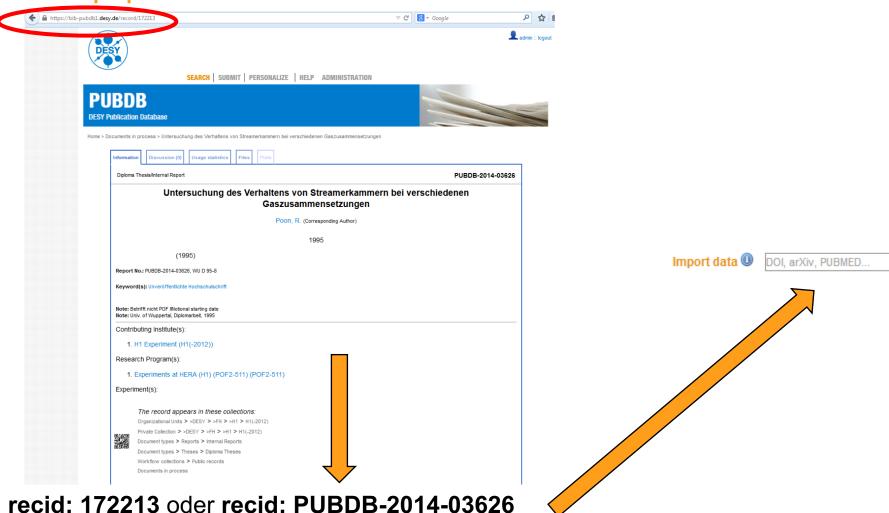
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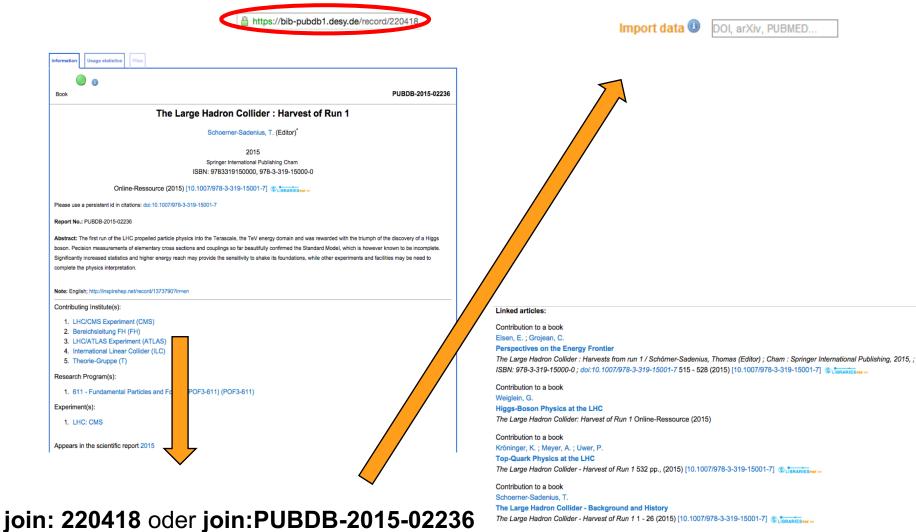


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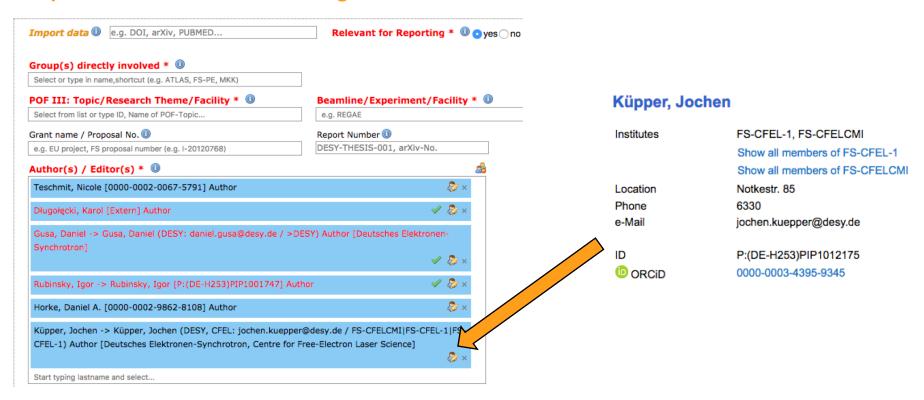
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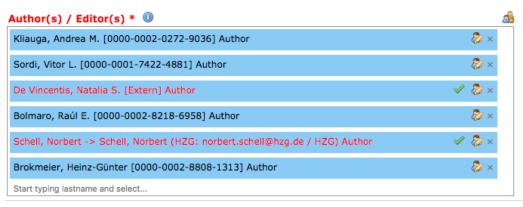
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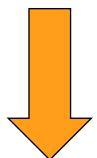
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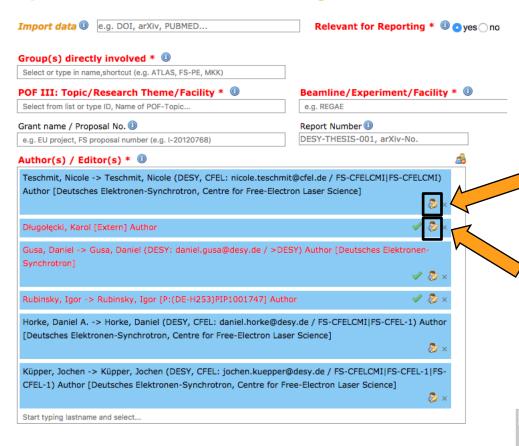
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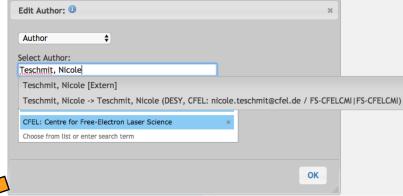
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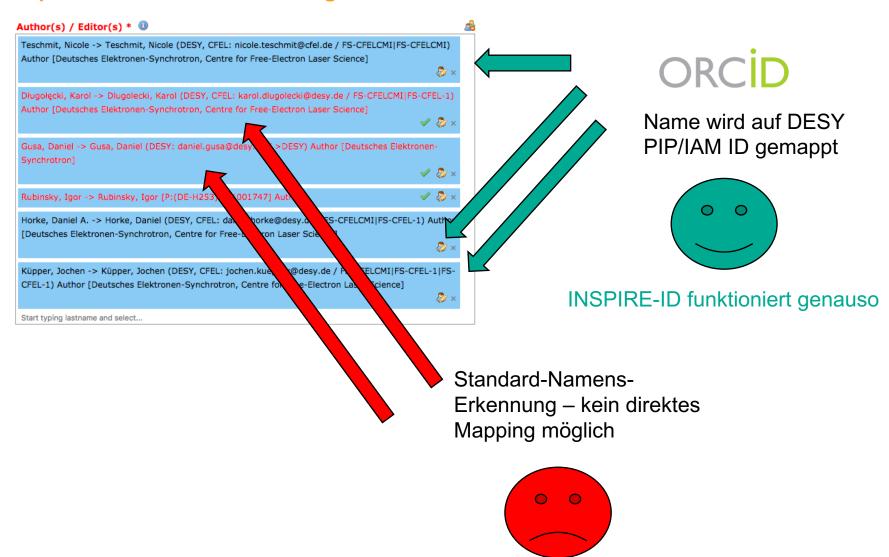
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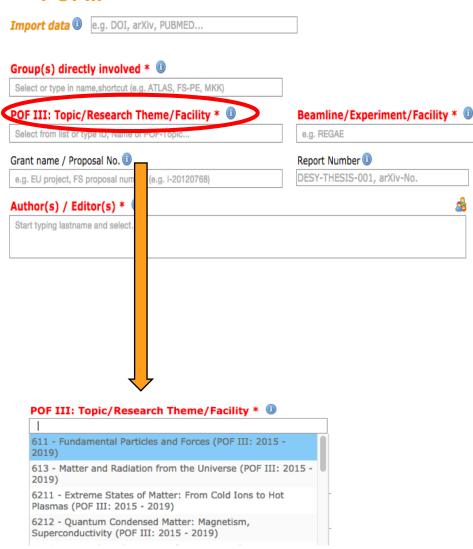
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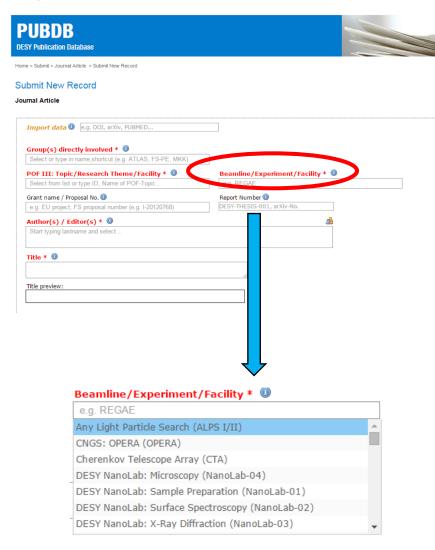
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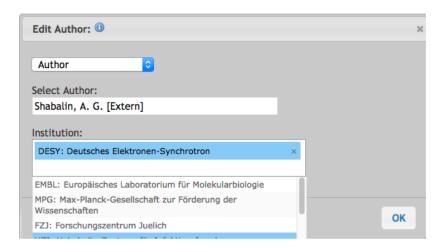
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[CMS-QCD-11-006; CERN-PH-EP-2014-302; arXiv:1502.04785]

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

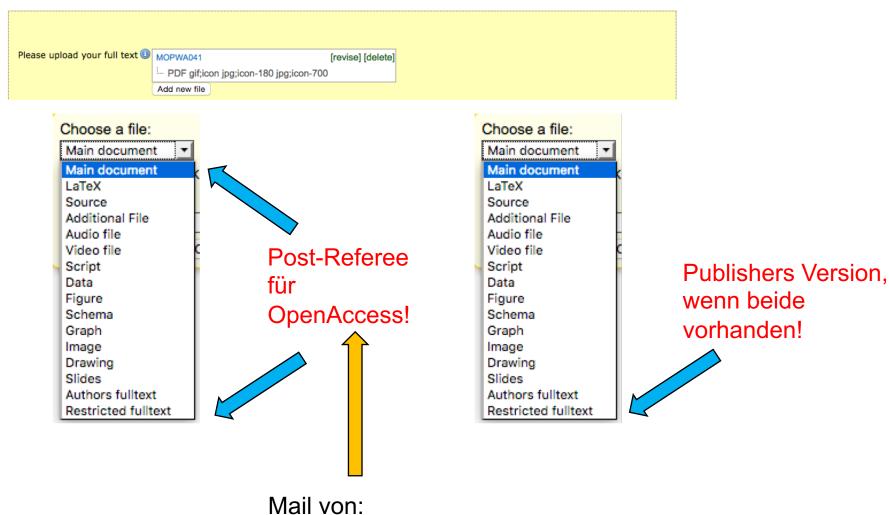
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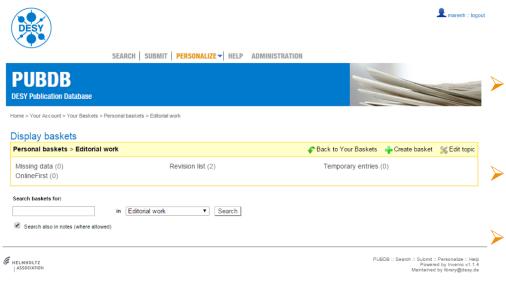
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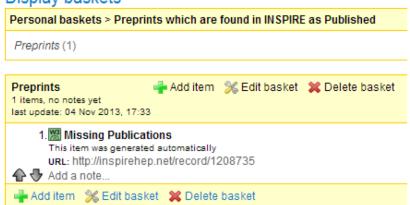
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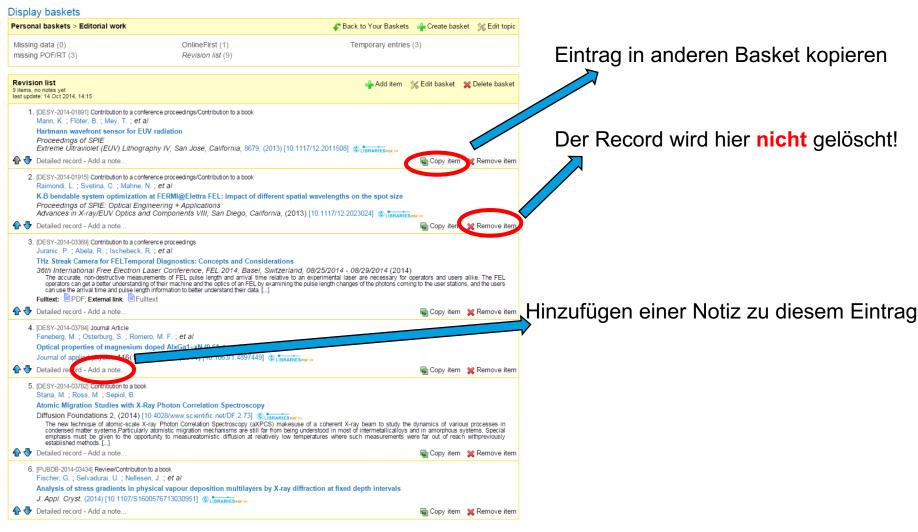
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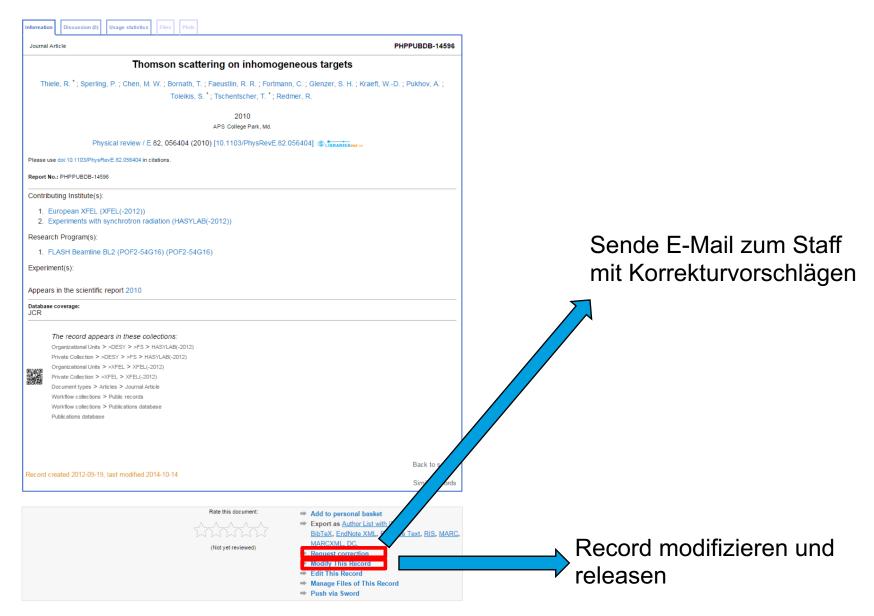


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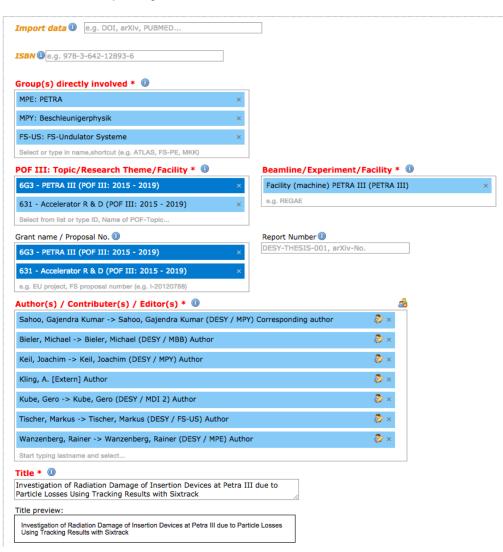
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Kienitz, J. S.; Dlugolecki, K.; Trippel, S. (Corresponding author); Küpper, J. (Corresponding author) Improved spatial separation of neutral molecules

The journal of chemical physics 147(2), 024304 (2017) [10.1063/1.4991479]

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Thesing, L. V.; Küpper, J. (Corresponding author); González-Férez, R. (Corresponding author) Time-dependent analysis of the mixed-field orientation of molecules without rotational symmetry The journal of chemical physics 146(24), 244304 (2017) [10.1063/1.4986954]

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Amini, K.; Boll, R.; Lauer, A.; Burt, M.; Lee, J. W. L.; Christensen, L.; Brauße, F.; Mullins, T.; Savelyev, E.; Ablikim, U.; Berrah, N.; Bomme, C.; Düsterer, S.; Erk, B.; Höppner, H.; Johnsson, P.; Kierspel, T.; Krecinic, F.; Küpper, J.; Müller, M.; Müller, E.; Redlin, H.; Rouzée, A.; Schirmel, N.; Thøgersen, J.; Techert, S.; Toleikis, S.; Treusch, R.; Trippel, S.; Ulmer, A.; Wiese, J.; Vallance, C.; Rudenko, A.; Stapelfeldt, H.; Brouard, M.; Rolles, D. (Corresponding author)
Alignment, orientation, and Coulomb explosion of difluoroiodobenzene studied with the pixel

imaging mass spectrometry (PImMS) camera

The journal of chemical physics 147(1), 013933 (2017) [10.1063/1.4982220]

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Savelyev, E.; Boll, R.; Bomme, C.; Schirmel, N.; Redlin, H.; Erk, B.; Düsterer, S.; Mueller, E.; Höppner, H.; Toleikis, S.; Müller, J.; Kristin Czwalinna, M.; Treusch, R.; Kierspel, T.; Mullins, T.; Trippel, S.; Wiese, J.; Küpper, J.; Brauße, F.; Krecinic, F.; Rouzée, A.; Rudawski, P.; Johnsson, P.; Amini, K.; Lauer, A.; Burt, M.; Brouard, M.; Christensen, L.; Thøgersen, J.; Stapelfeldt, H.; Berrah, N.; Müller, M.; Ulmer, A.; Techert, S.; Rudenko, A.; Rolles, D. (Corresponding author) Jitter-correction for IR/UV-XUV pump-probe experiments at the FLASH free-electron laser New journal of physics 19(4), 043009 (2017) [10.1088/1367-2630/aa652d]

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Owens, A. (Corresponding author); Zak, E. J.; Chubb, K. L.; Yurchenko, S. N.; Tennyson, J.; Yachmenev, A. (Corresponding author)

Simulating electric field interactions with polar molecules using spectroscopic databases Scientific reports 7, 45068 (2017) [10.1038/srep45068]

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Horke, D. (Corresponding author); Roth, N.; Worbs, L.; Küpper, J. Characterizing gas flow from aerosol particle injectors

Journal of applied physics 121(12), 123106 (2017) [10.1063/1.4978914]

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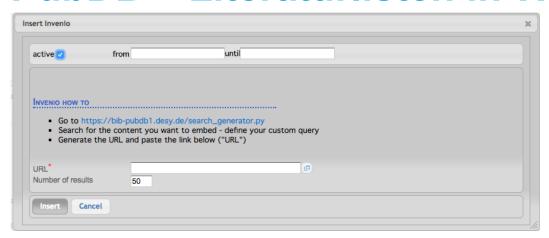
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Inducing Stable \alpha + \beta Microstructures during Selective Laser Melting of Ti-6Al-
4V Using Intensified Intrinsic Heat Treatments
Materials 10(3), 268 (2017) [10.3390/ma10030268]
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Intermetallics 82, 40 - 52 (2017) [10.1016/j.intermet.2016.11.003]
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Cao, H.; Guo, J.; Chang, F.; Pistidda, C.; Zhou, W.; Zhang, X.; Santoru, A.;
Wu, H.; Schell, N.; Niewa, R.; Chen, P.; Klassen, T.; Dornheim, M.
Transition and Alkali Metal Complex Ternary Amides for Ammonia Synthesis
and Decomposition
Chemistry - a European journal 23(41), 9766-9771 (2017) [10.1002/chem.201702728]
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Chen, Y.-H.; Rogström, L.; Roa, J. J.; Zhu, J. Q.; Schramm, I. C.; Johnson, L. J. S.;
Schell, N.; Mücklich, F.; Anglada, M. J.; Odén, M.
Thermal and mechanical stability of wurtzite-ZrAIN/cubic-TiN and wurtzite-
ZrAIN/cubic-ZrN multilayers
Surface and coatings technology 324, 328 - 337 (2017)
[10.1016/j.surfcoat.2017.05.055]
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Apaydin, D.; Böhm, A.; Rütt, U.; Bertram, F.; Hesser, G.; Scharber, M. C.;
Sariciftci, N. S.; Nickel, B.; Bauer, S.; Głowacki, E. D.; Kaltenbrunner, M.
Confining metal-halide perovskites in nanoporous thin films
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Science advances 3(8), e1700738 - (2017) [10.1126/sciadv.1700738]

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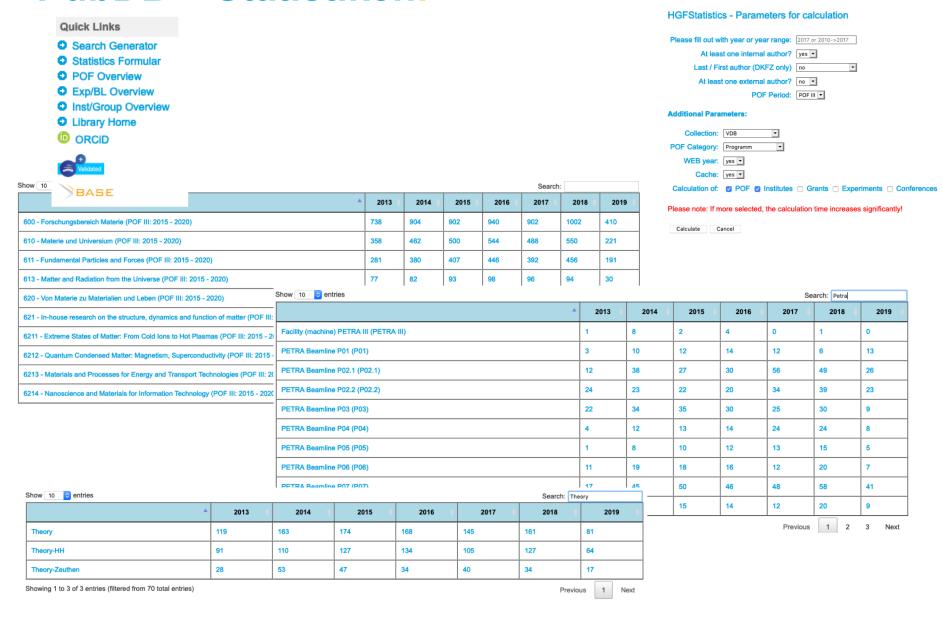
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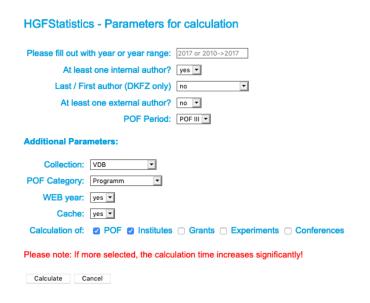
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A	WOS + Scopus (POFIII / POFIV Indikator)	WOS listed journal OR entry (POFII Indikator)	All of WoS and Scopus listed	Scopus listed	Thomson Reuters Master Journal List	JCR listed	WOS and not JCR	Web of Science	Other refereed	User supplied Peer Review	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)

Per institute and document type

Show 10 contries Search: Theory																
	A	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
Theory		4	0	93	4	1	0	0	87	0	179	4	37	47	0	8
Theory-	-нн	4	0	76	4	1	0	0	75	0	155	4	37	47	0	7
Theory- Zeuther		0	0	17	0	0	0	0	12	0	24	0	0	0	0	1

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

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.



- Implementierung von POFIV steht an, Erstellung der Normdatensätze, Erfassung von Altdaten, eventuelle zusätzliche POFIV-Maske, etc.
- Umstellung auf Docker zum leichteren Ausrollen unserer monatlichen Releases steht bevor
- Beginn der Invenio 3.x Migration?



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