Clas Persson

List of Publications by Year
in descending order

130 papers	5,601 citations	136950 32 h-index	85541 71 g-index
136 all docs	136 docs citations	136 times ranked	7194 citing authors

#	Article	IF	Citations
1	Electronic and optical properties of Cu2ZnSnS4 and Cu2ZnSnSe4. Journal of Applied Physics, 2010, 107, .	2.5	550
2	n-type doping ofCuInSe2andCuGaSe2. Physical Review B, 2005, 72, .	3.2	429
3	Anomalous Grain Boundary Physics in PolycrystallineCuInSe2: The Existence of a Hole Barrier. Physical Review Letters, 2003, 91, 266401.	7.8	305
4	Optical band-gap determination of nanostructured WO3 film. Applied Physics Letters, 2010, 96, .	3.3	281
5	Adsorption of metal adatoms on single-layer phosphorene. Physical Chemistry Chemical Physics, 2015, 17, 992-1000.	2.8	280
6	Strong Valence-Band Offset Bowing ofZnO1â^'xSxEnhancesp-Type Nitrogen Doping of ZnO-like Alloys. Physical Review Letters, 2006, 97, 146403.	7.8	245
7	The electronic structure of chalcopyritesâ€"bands, point defects and grain boundaries. Progress in Photovoltaics: Research and Applications, 2010, 18, 390-410.	8.1	237
8	Electronic structure of nanostructured ZnO from x-ray absorption and emission spectroscopy and the local density approximation. Physical Review B, 2004, 70, .	3.2	180
9	Cuâ€"Zn disorder and band gap fluctuations in Cu₂ZnSn(S,Se)₄: Theoretical and experimental investigations. Physica Status Solidi (B): Basic Research, 2016, 253, 247-254.	1.5	173
10	Metal-insulator transition and superconductivity in boron-doped diamond. Physical Review B, 2007, 75, .	3.2	162
11	Irvsp: To obtain irreducible representations of electronic states in the VASP. Computer Physics Communications, 2021, 261, 107760.	7.5	151
12	Comparative study of rutile and anatase SnO2 and TiO2: Band-edge structures, dielectric functions, and polaron effects. Journal of Applied Physics, 2013, 113, .	2.5	112
13	Band gap change induced by defect complexes in Cu2ZnSnS4. Thin Solid Films, 2013, 535, 265-269.	1.8	91
14	A computational study of Na behavior on graphene. Applied Surface Science, 2015, 333, 235-243.	6.1	90
15	Reducing the Charge Carrier Transport Barrier in Functionally Layerâ€Graded Electrodes. Angewandte Chemie - International Edition, 2017, 56, 14847-14852.	13.8	88
16	Lattice thermal conductivity of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ti</mml:mi><mml:mi>x</mml:mi></mml:ms alloys calculated from first principles: Key role of nature of phonon modes. Physical Review B, 2017, 95, .	3.2	79
17	Optical properties of Cu(In,Ga)Se2 and Cu2ZnSn(S,Se)4. Thin Solid Films, 2011, 519, 7508-7512.	1.8	77
18	Energy, Phonon, and Dynamic Stability Criteria of Two-Dimensional Materials. ACS Applied Materials & Interfaces, 2019, 11, 24876-24884.	8.0	76

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19	CuSbS2 and CuBiS2 as potential absorber materials for thin-film solar cells. Journal of Renewable and Sustainable Energy, 2013, 5, .	2.0	63
20	Dielectric function and double absorption onset of monoclinic Cu 2 SnS 3 : Origin of experimental features explained by first-principles calculations. Solar Energy Materials and Solar Cells, 2016, 154, 121-129.	6.2	62
21	The role of grain boundary scattering in reducing the thermal conductivity of polycrystalline XNiSn (Xâ€‰=â€‰Hf, Zr, Ti) half-Heusler alloys. Scientific Reports, 2017, 7, 13760.	3.3	55
22	Dielectric function spectra and critical-point energies of Cu2ZnSnSe4 from 0.5 to 9.0 eV. Journal of Applied Physics, 2012, 111, .	2.5	53
23	One step synthesis of pure cubic and monoclinic HfO2 nanoparticles: Correlating the structure to the electronic properties of the two polymorphs. Journal of Applied Physics, 2012, 112, .	2.5	52
24	Improved electronic structure and optical properties of sp-hybridized semiconductors using LDA+U SIC. Brazilian Journal of Physics, 2006, 36, 286-290.	1.4	50
25	Study of band-structure, optical properties and native defects in<i>A</i>^I<i>B</i>^{III}O₂(<i>A</i>^I= Cu or) Tj ETQq1 1 0.784314 rgBT /Overlock 10 065003.	2.0	49
26	Wideâ€gap (Ag,Cu)(In,Ga)Se₂ solar cells with different buffer materialsâ€"A path to a better heterojunction. Progress in Photovoltaics: Research and Applications, 2020, 28, 237-250.	8.1	47
27	Correlating the Peukertâ€™s Constant with Phase Composition of Electrode Materials in Fast Lithiation Processes. , 2019, 1, 519-525.		45
28	Electronic and optical properties of nanocrystalline WO₃thin films studied by optical spectroscopy and density functional calculations. Journal of Physics Condensed Matter, 2013, 25, 205502.	1.8	43
29	Hole-Doped 2D InSe for Spintronic Applications. ACS Applied Nano Materials, 2018, 1, 6656-6665.	5.0	41
30	Full-Spectrum High-Resolution Modeling of the Dielectric Function of Water. Journal of Physical Chemistry B, 2020, 124, 3103-3113.	2.6	35
31	Chemistry of Oxygen Ionosorption on SnO₂ Surfaces. ACS Applied Materials & Interfaces, 2021, 13, 33664-33676.	8.0	35
32	Optical properties and electronic structures of(4CuInSe2)y(CuIn5Se8)1â^'y. Physical Review B, 2006, 74, .	3.2	34
33	X-ray absorption and emission spectroscopy of ZnO nanoparticle and highly oriented ZnO microrod arrays. Microelectronics Journal, 2006, 37, 686-689.	2.0	34
34	Effective Polarizability Models. Journal of Physical Chemistry A, 2017, 121, 9742-9751.	2.5	33
35	Size effect on the conduction band orbital character of anatase TiO2 nanocrystals. Applied Physics Letters, 2011, 99, 183101.	3.3	32
36	In search of new reconstructions of (001) Î±-quartz surface: a first principles study. RSC Advances, 2014, 4, 55599-55603.	3.6	32

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37	Enhancement of thermoelectric properties by energy filtering: Theoretical potential and experimental reality in nanostructured ZnSb. Journal of Applied Physics, 2016, 119, .	2.5	31
38	Electronic and optical properties of Cu2<i>X</i>SnS4 (<i>X</i>â€‰=â€‰Be, Mg, Ca, Mn, Fe, and Ni) and the impact of native defect pairs. Journal of Applied Physics, 2017, 121, .	2.5	31
39	Stability and electronic properties of phosphorene oxides: from 0-dimensional to amorphous 2-dimensional structures. Nanoscale, 2017, 9, 2428-2435.	5.6	30
40	Novel semiconducting materials for optoelectronic applications: Al1â^'xTlxN alloys. Applied Physics Letters, 2008, 92, .	3.3	29
41	Casimir quantum levitation tuned by means of material properties and geometries. Physical Review B, 2014, 89, .	3.2	29
42	Thermodynamic stability, phase separation and Ag grading in (Ag,Cu)(In,Ga)Se₂ solar absorbers. Journal of Materials Chemistry A, 2020, 8, 8740-8751.	10.3	29
43	Temperature dependent band-gap energy for Cu2ZnSnSe4: A spectroscopic ellipsometric study. Solar Energy Materials and Solar Cells, 2014, 130, 375-379.	6.2	28
44	Optical properties of SiGe alloys. Journal of Applied Physics, 2003, 93, 3832-3836.	2.5	27
45	Spontaneous Non-stoichiometry and Ordering in Degenerate but Gapped Transparent Conductors. Matter, 2019, 1, 280-294.	10.0	27
46	Full band calculation of doping-induced band-gap narrowing inp-type GaAs. Physical Review B, 2001, 64, .	3.2	25
47	Understanding the optical properties of ZnO1â^'<i>x</i>S<i>x</i> and ZnO1â^'<i>x</i>Se<i>x</i> alloys. Journal of Applied Physics, 2016, 119, .	2.5	25
48	Tailoring electronic properties of multilayer phosphorene by siliconization. Physical Chemistry Chemical Physics, 2018, 20, 2075-2083.	2.8	25
49	Status of materials and device modelling for kesterite solar cells. JPhys Energy, 2019, 1, 042004.	5.3	24
50	Reducing the Charge Carrier Transport Barrier in Functionally Layerâ€Graded Electrodes. Angewandte Chemie, 2017, 129, 15043-15048.	2.0	23
51	Alkali Dispersion in (Ag,Cu)(In,Ga)Se₂ Thin Film Solar Cellsâ€"Insight from Theory and Experiment. ACS Applied Materials & Interfaces, 2021, 13, 7188-7199.	8.0	22
52	Surface studies of the chemical environment in gold nanorods supported by X-ray photoelectron spectroscopy (XPS) and ab initio calculations. Journal of Materials Research and Technology, 2021, 15, 768-776.	5.8	22
53	Distance-Dependent Sign Reversal in the Casimir-Lifshitz Torque. Physical Review Letters, 2018, 120, 131601.	7.8	21
54	Volume dependence of the dielectric properties of amorphous SiO₂. Physical Chemistry Chemical Physics, 2016, 18, 7483-7489.	2.8	20

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55	Strong Interplay between Sodium and Oxygen in Kesterite Absorbers: Complex Formation, Incorporation, and Tailoring Depth Distributions. Advanced Energy Materials, 2019, 9, 1900740.	19.5	20
56	Thermoelectric transport trends in group 4 half-Heusler alloys. Journal of Applied Physics, 2019, 126, .	2.5	20
57	Enhancement of ferromagnetic properties in Zn0.95Co0.05O nanoparticles by indium codoping: An experimental and theoretical study. Applied Physics Letters, 2010, 97, .	3.3	19
58	Band gap reduction and dielectric function of Ga_{1â^’<i>x</i>}Zn_{<i>x</i>}N_{1â^’<i>x</i>}O_{<i>x</i>} and In_{1â^’<i>x</i>}Zn_{<i>x</i>}N_{1â^’<i>x</i>}O_{<i>x</i>} alloys. Physica Status Solidi (A) Applications and Materials Science, 2012, 209, 75-78.	1.8	19
59	Effects of native defects on the structural and magnetic properties of hematite<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-Fe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:	3.2	19
60	Comparison of alpha and beta tin for lithium, sodium, and magnesium storage: An<i>ab initio</i>study including phonon contributions. Journal of Chemical Physics, 2015, 143, 204701.	3.0	19
61	High absorption coefficients of the CuSb(Se,Te)₂ and CuBi(S,Se)₂ alloys enable high-efficient 100 nm thin-film photovoltaics. EPJ Photovoltaics, 2017, 8, 85504.	1.6	19
62	Premelting of ice adsorbed on a rock surface. Physical Chemistry Chemical Physics, 2020, 22, 11362-11373.	2.8	19
63	Optical and reduced band gap inn- andp-type GaN and AlN. Journal of Applied Physics, 2002, 92, 3207-3216.	2.5	18
64	A full-band -method for solving the Kohnâ€“Sham equation. Computer Physics Communications, 2007, 177, 280-287.	7.5	18
65	Ice Particles Sink below the Water Surface Due to a Balance of Salt, van der Waals, and Buoyancy Forces. Journal of Physical Chemistry C, 2018, 122, 15311-15317.	3.1	18
66	Casimir force between atomically thin gold films. European Physical Journal B, 2013, 86, 1.	1.5	17
67	Band gap modulation of SrTiO₃ upon CO₂ adsorption. Physical Chemistry Chemical Physics, 2017, 19, 16629-16637.	2.8	17
68	First-Principles Mapping of the Electronic Properties of Two-Dimensional Materials for Strain-Tunable Nanoelectronics. ACS Applied Nano Materials, 2019, 2, 5614-5624.	5.0	17
69	ZnOâ€“InN nanostructures with tailored photocatalytic properties for overall water-splitting. International Journal of Hydrogen Energy, 2013, 38, 16727-16732.	7.1	16
70	Optical properties of Cu2ZnSn(SxSe1-x)4 solar absorbers: Spectroscopic ellipsometry and <i>ab initio</i> calculations. Applied Physics Letters, 2017, 110, .	3.3	16
71	Thermoelectric transport of GaAs, InP, and PbTe: Hybrid functional with kÂ·pÌƒ interpolation versus scissor-corrected generalized gradient approximation. Journal of Applied Physics, 2018, 123, .	2.5	16
72	Self-preserving ice layers on CO₂ clathrate particles: Implications for Enceladus, Pluto, and similar ocean worlds. Astronomy and Astrophysics, 2021, 650, A54.	5.1	16

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73	Cation vacancies in the alloy compounds of Cu2ZnSn(S1â˜Se)4 and CuIn(S1â˜Se)2. Thin Solid Films, 2013, 535, 318-321.	1.8	15
74	Optical absorption of rutile SnO2 and TiO2. Physica Status Solidi C: Current Topics in Solid State Physics, 2009, 6, 2740-2742.	0.8	14
75	Band-edge density-of-states and carrier concentrations in intrinsic and <i>p</i>-type CuIn1â˜<i>x</i>Ga<i>x</i>Se2. Journal of Applied Physics, 2012, 112, .	2.5	14
76	Casimir attractive-repulsive transition in MEMS. European Physical Journal B, 2012, 85, 1.	1.5	14
77	Evidence of defect band mechanism responsible for band gap evolution in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mo>(</mml:mo><mml:mi>ZnO</mml:mi><mml alloys. Physical Review B, 2019, 100, .	2.2	14
78	A photoelectron spectroscopy study of the electronic structure evolution in CuInSe₂-related compounds at changing copper content. Applied Physics Letters, 2012, 101, 111607.	3.3	13
79	Anisotropic contribution to the van der Waals and the Casimir-Polder energies for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>CO</mml:mtext><mml:mn>2</mml:mn></mml:msub xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>CH</mml:mtext><mml:mn>4</mml:mn></mml:msub [illegible] Physical Review A, 2015, 92.	2.5	13
80	Enabling accurate first-principle calculations of electronic properties with a corrected <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si3.gif" overflow="scroll"><mml:mrow><mml:mi mathvariant="bold">k</mml:mi><mml:mo>Â·</mml:mo><mml:mi mathvariant="bold">p</mml:mi></mml:mrow></mml:math> scheme. Computational Materials Science, 2017, 134, 17-24.	3.0	13
81	Suppression of surfaces states at cubic perovskite (001) surfaces by CO2 adsorption. Physical Chemistry Chemical Physics, 2018, 20, 18828-18836.	2.8	13
82	Structural, electronic and optical properties of silver delafossite oxides: A first-principles study with hybrid functional. Physica B: Condensed Matter, 2013, 422, 20-27.	2.7	12
83	Group-IV (Si, Ge, and Sn)-doped AgAlTe₂for intermediate band solar cell from first-principles study. Semiconductor Science and Technology, 2017, 32, 065007.	2.0	12
84	Fluid-sensitive nanoscale switching with quantum levitation controlled by <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î±</mml:mi></mml:math> -Sn/ <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î²</mml:mi></mml:math> -Sn phase transition. Physical Review B, 2018, 97, .	3.2	12
85	Ultrathin metallic coatings can induce quantum levitation between nanosurfaces. Applied Physics Letters, 2012, 100, 253104.	3.3	11
86	Investigation of the structural, optical and electronic properties of Cu₂Zn(Sn,Si/Ge)(S/Se)₄ alloys for solar cell applications. Physica Status Solidi (B): Basic Research, 2017, 254, 1700084.	1.5	11
87	Dispersion Forces Stabilize Ice Coatings at Certain Gas Hydrate Interfaces That Prevent Water Wetting. ACS Earth and Space Chemistry, 2019, 3, 1014-1022.	2.7	11
88	Casimir forces in a plasma: possible connections to Yukawa potentials. European Physical Journal D, 2014, 68, 1.	1.3	10
89	Exploring the electronic and optical properties of Cu₂Sn_{1<i>â˜x</i>}Ge_{<i>x</i>}S₃ and Cu₂Sn_{1â˜<i>x</i>}Si_{<i>x</i>}S₃ (<i>x</i>â€‰=â€‰0, 0.5, and 1). Physica Status Solidi (B): Basic Research, 2017, 254, 1700111.	1.5	10
90	Lifshitz interaction can promote ice growth at water-silica interfaces. Physical Review B, 2017, 95, .	3.2	10

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91	Intermolecular Casimir-Polder forces in water and near surfaces. Physical Review E, 2014, 90, 032122.	2.1	9
92	Noble gas as a functional dopant in ZnO. Npj Computational Materials, 2019, 5, .	8.7	9
93	Dispersion forces in inhomogeneous planarly layered media: A one-dimensional model for effective polarizabilities. Physical Review A, 2019, 99, .	2.5	8
94	Experimental and Theoretical Study of Stable and Metastable Phases in Sputtered CuInS₂. Advanced Science, 2022, 9, .	11.2	8
95	Density functional theory study of ordered defect Cu-(In,Ga)-Se compounds. Physica Status Solidi C: Current Topics in Solid State Physics, 2012, 9, 1600-1603.	0.8	7
96	Vacancy induced magnetism in WO3. European Physical Journal B, 2013, 86, 1.	1.5	7
97	The influence of Lifshitz forces and gas on premelting of ice within porous materials. Europhysics Letters, 2016, 115, 13001.	2.0	7
98	Effects of van der Waals forces and salt ions on the growth of water films on ice and the detachment of CO 2 bubbles. Europhysics Letters, 2016, 113, 43002.	2.0	7
99	Impact of effective polarisability models on the near-field interaction of dissolved greenhouse gases at ice and air interfaces. Physical Chemistry Chemical Physics, 2019, 21, 21296-21304.	2.8	7
100	Carrier-mediated ferromagnetism in two-dimensional PtS₂. RSC Advances, 2020, 10, 952-957.	3.6	7
101	Multiscale in modelling and validation for solar photovoltaics. EPJ Photovoltaics, 2018, 9, 10.	1.6	6
102	Interface of Sn-doped AgAlTe2 and LiInTe2: A theoretical model of tandem intermediate band absorber. Applied Physics Letters, 2021, 118, .	3.3	6
103	Premelting and formation of ice due to Casimir-Lifshitz interactions: Impact of improved parameterization for materials. Physical Review B, 2022, 105, .	3.2	6
104	Effects of Substrate and Postâ€Ðeposition Annealing on Structural and Optical Properties of (ZnO)_{1âˆ’<i>x</i>}(GaN)_{<i>x</i>} Films. Physica Status Solidi (B): Basic Research, 2019, 256, 1800529.	1.5	5
105	Nontrivial retardation effects in dispersion forces: From anomalous distance dependence to novel traps. Physical Review B, 2020, 101, .	3.2	5
106	Secondary ion mass spectrometry as a tool to study selenium gradient in Cu ₂ ZnSn(S,Se) ₄. Physica Status Solidi C: Current Topics in Solid State Physics, 2017, 14, 1600187.	0.8	5
107	Enlarged molecules from excited atoms in nanochannels. Physical Review A, 2012, 86, .	2.5	4
108	Optical characterization of ZnO nanopillars on Si and macroporous periodic Si structure. Journal of Applied Physics, 2012, 111, 123527.	2.5	4

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109	Orientational Dependence of the van der Waals Interactions for Finite-Sized Particles. Journal of Physical Chemistry A, 2018, 122, 4663-4669.	2.5	4
110	Thio-olivine Mn2SiS4 thin films by reactive magnetron sputtering: Structural and optical properties with insights from first principles calculations. Materials and Design, 2018, 152, 110-118.	7.0	4
111	Optical Properties of Cu₂ZnSn(S_{<i>x</i>}Se_{1â€‹<i>x</i>})₄ by Firstâ€Principles Calculations. Physica Status Solidi (A) Applications and Materials Science, 2018, 215, 1700945.	1.8	4
112	Effect of excess charge carriers and fluid medium on the magnitude and sign of the Casimir-Lifshitz torque. Physical Review B, 2019, 100, .	3.2	4
113	Long- and short-range structures of Ti_{1âˆ’x}Hf_xNi_{1.0/1.1}Sn half-Heusler compounds and their electric transport properties. CrystEngComm, 2019, 21, 3330-3342.	2.6	4
114	Dynamic Impurity Redistributions in Kesterite Absorbers. Physica Status Solidi (B): Basic Research, 2020, 257, 2000062.	1.5	4
115	Electronic and optical properties of rutile titanium dioxide. Physica Status Solidi C: Current Topics in Solid State Physics, 2004, 1, S241-S244.	0.8	3
116	Casimir-Lifshitz interaction between ZnO and SiO2nanorods in bromobenzene turns repulsive at intermediate separations due to retardation effects. Physical Review A, 2012, 85, .	2.5	3
117	Ternary Cu3BiY3 (Y = S, Se, and Te) for Thin-Film Solar Cells. Materials Research Society Symposia Proceedings, 2013, 1538, 235-240.	0.1	3
118	Increased porosity turns desorption to adsorption for gas bubbles near water-SiO2interface. Physical Review B, 2015, 91, .	3.2	3
119	Chemical stability of Ca₃Co_{4âˆ’x}O_{9+Î´}/CaMnO_{3âˆ’Î´} pâ€“n junction for oxide-based thermoelectric generators. RSC Advances, 2020, 10, 5026-5031.	3.6	3
120	Structural flyby characterization of nanoporosity. Physica Status Solidi C: Current Topics in Solid State Physics, 2004, 1, S277-S281.	0.8	2
121	n-type doping principles for doping CuInSe/sub 2/ and CuGaSe/sub 2/ with Cl, Br, I, Mg, Zn, and Cd. , 0, , .		2
122	Resonance interaction induced by metal surfaces catalyzes atom-pair breakage. Physical Review A, 2013, 87, .	2.5	2
123	Nonperturbative theory for the dispersion self-energy of atoms. Physical Review A, 2014, 90, .	2.5	2
124	Stoner Ferromagnetism in Hole-Doped CuM^{IIIA}O₂ with M^{IIIA} = Al, Ga, and In. ACS Applied Materials & Interfaces, 2021, 13, 29770-29779.	8.0	2
125	Morphology and Magnetic Coupling in ZnO:Co and ZnO:Ni Co-Doped with Li. Acta Physica Polonica A, 2011, 119, 95-98.	0.5	2
126	Spectroscopy of Nanoparticles without Light. Physical Review Applied, 2020, 13, .	3.8	1

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127	Fine structure in electronic transitions attributed to nitrogen donor in silicon carbide. Applied Physics Letters, 2021, 119, 262101.	3.3	1
128	Optical characterization of rocksalt Pb1-xSnxTe alloys. Physica Status Solidi (A) Applications and Materials Science, 2008, 205, 837-840.	1.8	0
129	Nanostructured ZnOâ€"X Alloys with Tailored Optoelectronic Properties for Solar-energy Technologies. Materials Research Society Symposia Proceedings, 2013, 1558, 1.	0.1	0
130	Improved theoretical model of InN optical properties. Physica Status Solidi C: Current Topics in Solid State Physics, 2014, 11, 581-584.	0.8	0