

# Stefano Leoni

## List of Publications by Year in descending order

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120  
papers

2,763  
citations

172207

29  
h-index

214527

47  
g-index

128  
all docs

128  
docs citations

128  
times ranked

3892  
citing authors

#	ARTICLE	IF	CITATIONS
1	Pressure-induced structural transformation of clathrate $\text{Ge}_{136}$ via ultrafast recrystallization of an amorphous intermediate. Physical Review B, 2022, 105, .		
2	Mechanisms of irreversible aquaporin-10 inhibition by organogold compounds studied by combined biophysical methods and atomistic simulations. Metallomics, 2021, 13, .	1.0	4
3	All-t2g Electronic Orbital Reconstruction of Monoclinic $\text{MoO}_2$ Battery Material. Applied Sciences (Switzerland), 2020, 10, 5730.	1.3	1
4	Pressure-induced orbital-selective metal from the Mott insulator $\text{BaFe}_2\text{As}_2$ . Physical Review B, 2020, 101, .		
5	Aquaporin-driven hydrogen peroxide transport: a case of molecular mimicry?. RSC Chemical Biology, 2020, 1, 390-394.	2.0	20
6	Harvesting Free Energy Landscapes in Biological Systems. Lecture Notes in Bioengineering, 2020, , 64-77.	0.3	0
7	Unveiling the Mechanisms of Aquaglyceroporinâ€³ Water and Glycerol Permeation by Metadynamics. Chemistry - A European Journal, 2019, 25, 8713-8718.	1.7	19
8	Structural tuning and catalysis of tungsten carbides for the regioselective cleavage of C O bonds. Journal of Catalysis, 2019, 369, 283-295.	3.1	38
9	Dynamic Displacement Disorder of Cubic $\text{BaTiO}_3$ . Physical Review Letters, 2018, 120, 167601.	2.9	25
10	Metashooting: a novel tool for free energy reconstruction from polymorphic phase transition mechanisms. Faraday Discussions, 2018, 211, 235-251.	1.6	5
11	Molecular Basis of Aquaporin-7 Permeability Regulation by pH. Cells, 2018, 7, 207.	1.8	30
12	Templated Chromophore Assembly on Peptide Scaffolds: A Structural Evolution. Chemistry - A European Journal, 2018, 24, 16136-16148.	1.7	16
13	On the Mechanism of Gold/NHC Compounds Binding to DNA Gâ€¢Quadruplexes: Combined Metadynamics and Biophysical Methods. Angewandte Chemie, 2018, 130, 14732-14736.	1.6	16
14	On the Mechanism of Gold/NHC Compounds Binding to DNA Gâ€¢Quadruplexes: Combined Metadynamics and Biophysical Methods. Angewandte Chemie - International Edition, 2018, 57, 14524-14528.	7.2	60
15	The ZIF system zinc(II) 4,5-dichoroimidazolate: theoretical and experimental investigations of the polymorphism and crystallization mechanisms. Zeitschrift Fur Kristallographie - Crystalline Materials, 2017, 232, 77-90.	0.4	7
16	The mechanism of aquaporin inhibition by gold compounds elucidated by biophysical and computational methods. Chemical Communications, 2017, 53, 3830-3833.	2.2	50
17	Selective orbital reconstruction in tetragonal $\text{FeS}$ : A density functional dynamical mean-field theory study. Scientific Reports, 2017, 7, 46439.	1.6	13
18	Microscopic description of insulator-metal transition in high-pressure oxygen. Scientific Reports, 2017, 7, 2632.	1.6	16

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19	Product tunable behavior of carbon nanotubes-supported Ni <sup>II</sup> -Fe catalysts for guaiacol hydrodeoxygenation. <i>Applied Catalysis A: General</i> , 2017, 529, 20-31.	2.2	153
20	Mechanism of Germacradien-4-ol Synthase-Controlled Water Capture. <i>Biochemistry</i> , 2016, 55, 2112-2121.	1.2	25
21	Enzymatic synthesis of natural (+)-aristolochene from a non-natural substrate. <i>Chemical Communications</i> , 2016, 52, 14027-14030.	2.2	6
22	Hierarchical thermoelectrics: crystal grain boundaries as scalable phonon scatterers. <i>Nanoscale</i> , 2016, 8, 3729-3738.	2.8	17
23	A zeolitic imidazolate framework with conformational variety: conformational polymorphs versus frameworks with static conformational disorder. <i>CrystEngComm</i> , 2016, 18, 2477-2489.	1.3	26
24	Magnetoresistance in the Spin-Orbit Kondo State of Elemental Bismuth. <i>Scientific Reports</i> , 2015, 5, 13772.	1.6	13
25	Microwave-Assisted Synthesis of Defects Metal-Imidazolate-Amide-Imidate Frameworks and Improved CO <sub>2</sub> Capture. <i>Inorganic Chemistry</i> , 2015, 54, 10073-10080.	1.9	27
26	Atomistic modeling of diffuse scattering in cubic PbZrO <sub>3</sub> . <i>Phase Transitions</i> , 2015, 88, 273-282.	0.6	20
27	Orbital-selective Mottness in layered iron oxychalcogenides: the case of Na <sub>2</sub> Fe <sub>2</sub> OSe <sub>2</sub> . <i>Journal of Physics Condensed Matter</i> , 2014, 26, 145602.	0.7	9
28	Novel Carbons: Habits and Oddities. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2014, 640, 681-688.	0.6	5
29	The rules of metastability: detailed transformation mechanisms in chemical elements by means of molecular dynamics techniques. <i>Chemical Modelling</i> , 2014, , 30-56.	0.2	0
30	Zeolitic imidazolate framework-71 nanocrystals and a novel SOD-type polymorph: solution mediated phase transformations, phase selection via coordination modulation and a density functional theory derived energy landscape. <i>Dalton Transactions</i> , 2014, 43, 3528.	1.6	52
31	Metastable metal imidazolates: development of targeted syntheses by combining experimental and theoretical investigations of the formation mechanisms. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2014, 229, 807-822.	0.4	9
32	Indium Imidazolate Frameworks with Differently Distorted ReO <sub>3</sub> -Type Structures: Syntheses, Structures, Phase Transitions, and Crystallization Studies. <i>Crystal Growth and Design</i> , 2014, 14, 4664-4673.	1.4	11
33	Novel metastable metallic and semiconducting germaniums. <i>Scientific Reports</i> , 2013, 3, 1466.	1.6	31
34	A two-electron mechanism of lithium insertion into layered $\hat{I}\pm$ -MoO <sub>3</sub> : a DFT and DFT+U study. <i>Journal of Materials Chemistry A</i> , 2013, 1, 1778-1784.	5.2	46
35	Subtle polymorphism of zinc imidazolate frameworks: temperature-dependent ground states in the energy landscape revealed by experiment and theory. <i>CrystEngComm</i> , 2013, 15, 4036-4040.	1.3	38
36	Theoretical investigation of the electronic structure and quantum transport in the graphene <sup>II</sup> C(111) diamond surface system. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 435302.	0.7	13

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37	Kondoesque origin of resistivity anisotropy in graphite. Physical Review B, 2013, 87, .	1.1	13
38	Redesign of Carbon Materials for Novel Storage, Mechanical and Optical Properties. Materials Research Society Symposia Proceedings, 2012, 1451, 9-14.	0.1	0
39	Squeezing lone pairs: The $A_{17}$ to $A_7$ pressure-induced phase transition in black phosphorus. Physical Review B, 2012, 85, .	1.1	81
40	Materials for Lithium Ion Batteries: Challenges for Numerical Simulations. Zeitschrift Fur Physikalische Chemie, 2012, 226, 95-106.	1.4	4
41	Framework reconstruction between hR8 and cI16 germaniums: A molecular dynamics study. RSC Advances, 2012, 2, 8833.	1.7	3
42	Bulk quantum correlations and doping-induced nonmetallicity in the $Bi_2Se_3$ family of topological insulators. Physical Review B, 2012, 85, .	1.1	13
43	Uniaxial $Bi_2Te_3$ and $Bi_2Se_3$ as topological insulators. Physical Review B, 2012, 85, .	1.1	14
44	Materials for Lithium Ion Batteries: Challenges for Numerical Simulations. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2012, 638, 1555-1555.	0.6	0
45	Reticular Materials for Hydrogen Storage. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2012, 638, 1626-1626.	0.6	0
46	Redesign of Carbon Materials for Novel Storage, Mechanical and Optical Properties. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2012, 638, 1626-1626.	0.6	0
47	Electron localization in olivine materials for advanced lithium-ion batteries. Journal of Applied Physics, 2012, 111, 112602.	1.1	6
48	Understanding the nature of "superhard graphite". Scientific Reports, 2012, 2, 471.	1.6	86
49	An Isorecticular Family of Microporous Metal-Organic Frameworks Based on Zinc and Substituted Imidazolate-Amide-Imidate: Syntheses, Structures and Properties. Chemistry - A European Journal, 2012, 18, 11630-11640.	1.7	26
50	The energy landscapes of zeolitic imidazolate frameworks (ZIFs): towards quantifying the presence of substituents on the imidazole ring. Journal of Materials Chemistry, 2012, 22, 10152-10154.	6.7	29
51	Polymorphs of lithium-boron imidazolates: energy landscape and hydrogen storage properties. Dalton Transactions, 2011, 40, 3796-3798.	1.6	22
52	Electrodynamics and quantum capacity of $Li_xFePO_4$ battery material. Applied Physics Letters, 2011, 99, 192103.	1.5	12
53	Superhard $s_p^3$ allotropes with odd and even ring topologies. Physical Review B, 2011, 84, .	1.1	9
54	Atomistic investigation of $Li^+$ diffusion pathways in the olivine $LiFePO_4$ cathode material. Journal of Materials Chemistry, 2011, 21, 16365.	6.7	42

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55	On the continuous transformations between genus-3 minimal surfaces approximants. Zeitschrift Für Kristallographie, 2011, 226, 678-683.	1.1	3
56	A Walk on the Chemical Landscape: The Role of B33 along the B1â€“B2 Phase Transition in RbF and NaBr. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2011, 637, 864-869.	0.6	3
57	Packings of Carbon Nanotubes â€“ New Materials for Hydrogen Storage. Advanced Materials, 2011, 23, 1237-1241.	11.1	76
58	Route to a Family of Robust, Nonâ€“interpenetrated Metalâ€“Organic Frameworks with ptoâ€“like Topology. Chemistry - A European Journal, 2011, 17, 13007-13016.	1.7	127
59	Hydrogen storage in zeolite imidazolate frameworks. A multiscale theoretical investigation. International Journal of Hydrogen Energy, 2011, 36, 6005-6013.	3.8	38
60	Unconventional Mott transition in $KxFe_2Se_2$ . Physical Review B, 2011, 84, .	1.1	29
61	Novel Computational Approaches to Li Diffusion and Electron Transport for High Capacity Battery Materials. Materials Research Society Symposia Proceedings, 2011, 1313, 70101.	0.1	0
62	Structural transitions in solids. Acta Crystallographica Section A: Foundations and Advances, 2010, 66, 505-506.	0.3	0
63	Subtle Polymorphism in the Zinc Imidazolate System. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2010, 636, 2086-2086.	0.6	2
64	Local structure in the paraelectric phase of $Cd_2In_4S_8$ from x-ray diffuse scattering, by means of <i>ab initio</i> molecular dynamics and Monte Carlo modeling. Physical Review B, 2010, 81, .	1.1	18
65	Low-temperature metal-insulator transition in the electron-doped iron chalcogenide FeSe superconductor. Europhysics Letters, 2010, 91, 27001.	0.7	19
66	Comparative study of tetragonal and hexagonal FeSe: An orbital-selective scenario. Europhysics Letters, 2010, 92, 67003.	0.7	26
67	Atomistic engineering in the control of the electronic properties of CdSe nanotubes. Physical Review B, 2010, 82, .	1.1	4
68	Modelling polymorphs of metalâ€“organic frameworks: a systematic study of diamondoid zinc imidazolates. CrystEngComm, 2010, 12, 2809.	1.3	25
69	Hydrogen Adsorption Sites in Zeolite Imidazolate Frameworks ZIF-8 and ZIF-11. Journal of Physical Chemistry C, 2010, 114, 13381-13384.	1.5	66
70	Polarized Cluster Dynamics at the Paraelectric to Ferroelectric Phase Transition in $BaTiO_3$ . Journal of Physical Chemistry B, 2010, 114, 16465-16470.	1.2	17
71	Electrodynamic response of incoherent metals: Normal phase of iron pnictides. Physical Review B, 2009, 79, .	1.1	29
72	Self-doping induced orbital-selective Mott transition in $Hg_2Ru_2O_7$ . Physical Review B, 2009, 79, .	1.1	10

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73	$\text{Ca}_3\text{N}_2$ , a Metastable Nitride in the System $\text{Ca-N}$ . Chemistry - A European Journal, 2009, 15, 3419-3425.	1.7	17
74	Deconstructing Sodalite with Hyperbolic Tilings: A PNS Approach. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2009, 635, 619-623.	0.6	1
75	$\text{VNb}_9\text{O}_{25}$ Synthesis, electrical conducting behaviour and density functional theory (DFT) calculation. Journal of Solid State Chemistry, 2009, 182, 2053-2060.	1.4	12
76	GerÃ¼stverbindungen mit beweglichen Lanthan(III)-Eisen(II)-Sulfid-Halogenide $\text{La}_3\text{Fe}_2\text{S}_9\text{OX}_3$ (X = Cl, Br, I). Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2008, 634, 107-114.	0.6	2
77	The Role of Interfaces in Ionic Conductors and Ferroelectrics. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2008, 634, 2013-2013.	0.6	0
78	Enumeration of Not-Yet-Synthesized Zeolitic Zinc Imidazolate MOF Networks: A Topological and DFT Approach. Journal of Physical Chemistry B, 2008, 112, 9437-9443.	1.2	93
79	Competing intermediates in the pressure-induced wurtzite to rocksalt phase transition in ZnO. Physical Review B, 2008, 78, .	1.1	33
80	Normal-state correlated electronic structure of iron pnictides from first principles. Physical Review B, 2008, 78, .	1.1	73
81	Theory of the orbital-selective Mott transition in ferromagnetic $\text{YTiO}_3$ under high pressure. Physical Review B, 2008, 77, .	1.1	7
82	Nanodomain fragmentation and local rearrangements in CdSe under pressure. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 19612-19616.	3.3	27
83	Orbital-spin order and the origin of structural distortion in $\text{MgTi}_2\text{O}_7$ . Physical Review B, 2008, 78, .	1.1	25
84	Walking the Path from B4- to B1-Type Structures in GaN. Physical Review Letters, 2007, 99, 125505.	2.9	46
85	Orbital-selective charge dynamics in $\text{YTiO}_3$ across the magnetic transition: Combined local-density approximation and dynamical mean-field theory. Physical Review B, 2007, 76, .	1.1	8
86	Microscopic Mechanism and Domain Formation in the Paraelectric to Ferroelectric Phase Transitions in $\text{BaTiO}_3$ . Materials Research Society Symposia Proceedings, 2007, 1034, 84.	0.1	0
87	Solid-Solid Phase Transitions: Interface Controlled Reactivity and Formation of Intermediate Structures. Chemistry - A European Journal, 2007, 13, 10022-10029.	1.7	16
88	Formation, Structure, and Polymorphism of Novel Lowest-Dimensional AgI Nanoaggregates by Encapsulation in Carbon Nanotubes. Small, 2007, 3, 1730-1734.	5.2	21
89	Extending the scope of <i>in silico</i> experiments™: Theoretical approaches for the investigation of reaction mechanisms, nucleation events and phase transitions. Science and Technology of Advanced Materials, 2007, 8, 434-441.	2.8	10
90	Low-dimensional sublattice melting by pressure: Superionic conduction in the phase interfaces of the fluorite-to-cotunnite transition of $\text{CaF}_2$ . Physical Review B, 2006, 74, .	1.1	30

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91	Mechanisms and Nucleation Characteristics of the Pressure-Induced B1 $\rightarrow$ B2 Transition in Potassium Halides: A Question of Ion Hardness and Softness. <i>Journal of Physical Chemistry B</i> , 2006, 110, 10873-10877.	1.2	15
92	Full-Featured Simulation of Reconstructive Solid-Solid Phase Transitions. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2006, 632, 2086-2086.	0.6	0
93	The role of covalency in the orbital-order of 3d1 perovskites. <i>Solid State Sciences</i> , 2006, 8, 1138-1143.	1.5	10
94	High-pressure crystal chemistry of binary intermetallic compounds. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2006, 221, 420-434.	0.4	46
95	Publisher's Note: Low-dimensional sublattice melting by pressure: Superionic conduction in the phase interfaces of the fluorite-to-cotunnite transition of CaF <sub>2</sub> [Phys. Rev. B74, 094106 (2006)]. <i>Physical Review B</i> , 2006, 74, .	1.1	0
96	Hidden orbital fluctuations in the solid solution Y <sub>1-x</sub> La <sub>x</sub> TiO <sub>3</sub> (x < 0.2). <i>Physical Review B</i> , 2006, 74, .	1.1	10
97	Novel Barium Beryllates Ba[Be <sub>2</sub> N <sub>2</sub> ] and Ba <sub>3</sub> [Be <sub>5</sub> O <sub>8</sub> ]: Syntheses, Crystal Structures and Bonding Properties.. <i>ChemInform</i> , 2005, 36, no.	0.1	0
98	Novel Barium Beryllates Ba[Be <sub>2</sub> N <sub>2</sub> ] and Ba <sub>3</sub> [Be <sub>5</sub> O <sub>8</sub> ]: Syntheses, Crystal Structures and Bonding Properties. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2005, 631, 1818-1824.	0.6	13
99	Multicenter multidomain B1 $\rightarrow$ B2 pressure-induced reconstructive phase transition in potassium fluoride. <i>Physical Review B</i> , 2005, 72, .	1.1	23
100	Mechanism of the pressure-induced wurtzite to rocksalt transition of CdSe. <i>Physical Review B</i> , 2005, 72, .	1.1	52
101	Putting the squeeze on NaCl: modelling and simulation of the pressure driven B1-B2 phase transition. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2004, 219, 339-344.	0.4	28
102	Insulator-metal transition in the doped 3d1 transition metal oxide LaTiO <sub>3</sub> . <i>Physical Review B</i> , 2004, 70, .	1.1	38
103	Ae[Be <sub>2</sub> N <sub>2</sub> ]: Nitridoberyllates of the Heavier Alkaline-Earth Metals. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 1088-1092.	7.2	15
104	Ae[Be <sub>2</sub> N <sub>2</sub> ]: Nitridoberyllates of the Heavier Alkaline-Earth Metals.. <i>ChemInform</i> , 2004, 35, no.	0.1	0
105	Nucleation and Growth in Pressure-Induced Phase Transitions from Molecular Dynamics Simulations: Mechanism of the Reconstructive Transformation of NaCl to the CsCl-Type Structure. <i>Physical Review Letters</i> , 2004, 92, 250201.	2.9	79
106	Mechanism of the pressure induced reconstructive transformation of KCl from the NaCl type to the CsCl type structure. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2004, 219, .	0.4	12
107	Elucidation of simple pathways for reconstructive phase transitions using periodic equi-surfaces (PES) descriptors. II. The strontium disilicide transition. <i>Solid State Sciences</i> , 2003, 5, 95-107.	1.5	4
108	BaAl <sub>2</sub> Ge <sub>2</sub> : synthesis, crystal structure, magnetic and electronic properties, chemical bonding, and atomistic model of the $\Gamma_2^{\pm}$ phase transition. <i>Solid State Sciences</i> , 2003, 5, 139-148.	1.5	20

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109	Modelling of the $\hat{I}_{\pm}$ (Clathrate VIII) $\leftrightarrow$ $\hat{I}_{\pm}^2$ (Clathrate I) Phase Transition in $\text{Eu}_8\text{Ga}_{16}\text{Ge}_{30}$ .. ChemInform, 2003, 34, no.	0.1	0
110	$\text{BaAl}_2\text{Ge}_2$ : Synthesis, Crystal Structure, Magnetic and Electronic Properties, Chemical Bonding, and Atomistic Model of the $\hat{I}_{\pm} \leftrightarrow \hat{I}_{\pm}^2$ Phase Transition.. ChemInform, 2003, 34, no.	0.1	0
111	$\text{Li}_3[\text{ScN}_2]$ : The First Nitridoscandate(III) $\leftrightarrow$ Tetrahedral Sc Coordination and Unusual $\text{MX}_2$ Framework.. ChemInform, 2003, 34, no.	0.1	0
112	$\text{Li}_3[\text{ScN}_2]$ : The First Nitridoscandate(III) $\leftrightarrow$ Tetrahedral Sc Coordination and Unusual $\text{MX}_2$ Framework. Chemistry - A European Journal, 2003, 9, 4255-4259.	1.7	15
113	Modelling of the $\hat{I}_{\pm}$ (clathrate VIII) $\leftrightarrow$ $\hat{I}_{\pm}^2$ (clathrate I) phase transition in $\text{Eu}_8\text{Ga}_{16}\text{Ge}_{30}$ . Journal of Alloys and Compounds, 2003, 350, 113-122.	2.8	31
114	Chemical, thermal, and theoretical analysis of the $\hat{I}_{\pm} \leftrightarrow \hat{I}_{\pm}^2$ phase transition of $\text{Ba}_3\text{Tt}_4$ compounds. Zeitschrift Fur Kristallographie - Crystalline Materials, 2003, 218, 171-177.	0.4	4
115	$\text{Zn}_3(\text{C}_6\text{H}_{14}\text{N}_2)_3[\text{B}_6\text{P}_{12}\text{O}_{39}(\text{OH})_{12}] \leftrightarrow \text{S} \cdot \text{S}(\text{C}_6\text{H}_{14}\text{N}_2)[\text{HPO}_4]$ : A Chiral Borophosphate - Triethylenediammonium Hydrogenphosphate Composite. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2002, 628, 67-76.	0.6	24
116	On Tilings and Patterns on Hyperbolic Surfaces and Their Relation to Structural Chemistry. ChemPhysChem, 2001, 2, 413-422.	1.0	31
117	On Tilings and Patterns on Hyperbolic Surfaces and Their Relation to Structural Chemistry. , 2001, 2, 413.		2
118	$\text{Ce}_4[\text{Si}_4\text{O}_4\text{N}_6]\text{O}$ -A Hyperbolically Layered Oxonitridosilicate Oxide with an Ordered Distribution of Oxygen and Nitrogen. Chemistry - A European Journal, 2000, 6, 2714-2720.	1.7	47
119	Structure and Reactivity of $[\text{Mo}_3\text{S}_4\text{S}-(\text{S})_3]^{4+}$ Complexes. Quantum Chemical Calculations, X-ray Structural Characterization, and Raman Spectroscopic Measurements. Inorganic Chemistry, 1998, 37, 2633-2644.	1.9	45
120	$\text{PbTe}/\text{PbSe}$ Thermoelectric Nanocomposites: The Impact of Length Modulations on Lowering Thermal Conductivity. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 0, , .	0.6	2