Davide Donadio

List of Publications by Year
in descending order

149 papers	21,746 citations	41258 49 h-index	9553 142 g-index
154 all docs	154 docs citations	154 times ranked	24394 citing authors

#	Article	IF	Citations
1	Evolution of structure and transport properties of the Ba8Cu16P30 clathrate-I framework with the introduction of Ga. Applied Physics Letters, 2022, 120, .	1.5	2
2	Enhanced photodegradation of dimethoxybenzene isomers in/on ice compared to in aqueous solution. Atmospheric Chemistry and Physics, 2022, 22, 5943-5959.	1.9	5
3	Effect of crystallinity and thickness on thermal transport in layered PtSe2. Npj 2D Materials and Applications, 2022, 6, .	3.9	12
4	Barbalinardo etÂal. Reply:. Physical Review Letters, 2022, 128, .	2.9	2
5	Synergistic impeding of phonon transport through resonances and screw dislocations. Physical Review B, 2021, 103, .	1.1	16
6	Ultrahigh Convergent Thermal Conductivity of Carbon Nanotubes from Comprehensive Atomistic Modeling. Physical Review Letters, 2021, 127, 025902.	2.9	18
7	Solid Solution Yb2â€“xCaxCdSb2: Structure, Thermoelectric Properties, and Quality Factor. Inorganic Chemistry, 2021, 60, 13596-13606.	1.9	11
8	Direct observation of ultrafast hydrogen bond strengthening in liquid water. Nature, 2021, 596, 531-535.	13.7	53
9	Mode localization and suppressed heat transport in amorphous alloys. Physical Review B, 2021, 103, .	1.1	12
10	Unprecedented superstructure in the type I family of clathrates. Chemical Communications, 2021, 57, 13780-13783.	2.2	3
11	Engineering Thermal Transport across Layered Grapheneâ€“MoS₂ Superlattices. ACS Nano, 2021, 15, 19503-19512.	7.3	16
12	Thermal transport in amorphous small organic materials: a mechanistic study. Physical Chemistry Chemical Physics, 2020, 22, 3058-3065.	1.3	16
13	IIIâ€“V Clathrate Semiconductors with Outstanding Hole Mobility: Cs8In27Sb19 and A8Ga27Sb19 (A = Cs,) Tj ETQq1 1 0.784314 rgB	6.6	27
14	Atomistic simulations of thermal conductivity in GeTe nanowires. Journal Physics D: Applied Physics, 2020, 53, 054001.	1.3	20
15	Mn-intercalated MoSe2 under pressure: Electronic structure and vibrational characterization of a dilute magnetic semiconductor. Journal of Chemical Physics, 2020, 153, 124701.	1.2	5
16	Efficient anharmonic lattice dynamics calculations of thermal transport in crystalline and disordered solids. Journal of Applied Physics, 2020, 128, .	1.1	22
17	Transferability of neural network potentials for varying stoichiometry: Phonons and thermal conductivity of MnxGey compounds. Journal of Applied Physics, 2020, 127, .	1.1	27
18	Photodecay of guaiacol is faster in ice, and even more rapid on ice, than in aqueous solution. Environmental Sciences: Processes and Impacts, 2020, 22, 1666-1677.	1.7	14

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19	Anisotropic In-Plane Phonon Transport in Silicon Membranes Guided by Nanoscale Surface Resonators. Physical Review Applied, 2020, 14, .	1.5	14
20	Beating the Thermal Conductivity Alloy Limit Using Long-Period Compositionally Graded Si_{1â€“x}Ge_x Superlattices. Journal of Physical Chemistry C, 2020, 124, 19864-19872.	1.5	9
21	Bathochromic Shift in the UVâ€“Visible Absorption Spectra of Phenols at Ice Surfaces: Insights from First-Principles Calculations. Journal of Physical Chemistry A, 2020, 124, 9288-9298.	1.1	14
22	Carbon dioxide, bicarbonate and carbonate ions in aqueous solutions under deep Earth conditions. Physical Chemistry Chemical Physics, 2020, 22, 10717-10725.	1.3	10
23	Thermal Transport: Overview. , 2020, , 723-733.		0
24	Promoting transparency and reproducibility in enhanced molecular simulations. Nature Methods, 2019, 16, 670-673.	9.0	655
25	Modeling heat transport in crystals and glasses from a unified lattice-dynamical approach. Nature Communications, 2019, 10, 3853.	5.8	122
26	Structural Complexity and High Thermoelectric Performance of the Zintl Phase: Yb₂₁Mn₄Sb₁₈. Chemistry of Materials, 2019, 31, 8076-8086.	3.2	28
27	Energy Relaxation and Thermal Diffusion in Infrared Pumpâ€“Probe Spectroscopy of Hydrogen-Bonded Liquids. Journal of Physical Chemistry Letters, 2019, 10, 3447-3452.	2.1	10
28	Hybrid Materials: Flexible and Ultrasoft Inorganic 1D Semiconductor and Heterostructure Systems Based on SnIP (Adv. Funct. Mater. 18/2019). Advanced Functional Materials, 2019, 29, 1970120.	7.8	0
29	Flexible and Ultrasoft Inorganic 1D Semiconductor and Heterostructure Systems Based on SnIP. Advanced Functional Materials, 2019, 29, 1900233.	7.8	37
30	Advances in the optimization of silicon-based thermoelectrics: a theory perspective. Current Opinion in Green and Sustainable Chemistry, 2019, 17, 35-41.	3.2	5
31	Quasi-Ballistic Thermal Transport Across MoS₂ Thin Films. Nano Letters, 2019, 19, 2434-2442.	4.5	61
32	Strongly tunable anisotropic thermal transport in MoS ₂ by strain and lithium intercalation: first-principles calculations. 2D Materials, 2019, 6, 025033.	2.0	31
33	Influence of thermostatting on nonequilibrium molecular dynamics simulations of heat conduction in solids. Journal of Chemical Physics, 2019, 151, 234105.	1.2	126
34	Thermal transport across graphene step junctions. 2D Materials, 2019, 6, 011005.	2.0	15
35	Efficient thermal diode with ballistic spacer. Physical Review E, 2018, 97, 030101.	0.8	20
36	Decisive role of nuclear quantum effects on surface mediated water dissociation at finite temperature. Journal of Chemical Physics, 2018, 148, 102320.	1.2	32

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37	High Seebeck Coefficient and Unusually Low Thermal Conductivity Near Ambient Temperatures in Layered Compound Yb_{2â€“x}Eu_xCdSb₂. Chemistry of Materials, 2018, 30, 484-493.	3.2	45
38	Selective adsorption of a supramolecular structure on flat and stepped gold surfaces. Surface Science, 2018, 670, 44-50.	0.8	3
39	Thermal transport in finite-size van der Waals materials: Modeling and Simulations. , 2018, , .		1
40	Structure and Dynamics of the Quasi-Liquid Layer at the Surface of Ice from Molecular Simulations. Journal of Physical Chemistry C, 2018, 122, 24780-24787.	1.5	38
41	Thermal Transport: Overview. , 2018, , 1-11.		2
42	An electrochemical thermal transistor. Nature Communications, 2018, 9, 4510.	5.8	105
43	Enhanced thermoelectric performance of two dimensional MS2 (MÂ=ÂMo, W) through phase engineering. Journal of Materiomics, 2018, 4, 329-337.	2.8	21
44	Simulating Energy Relaxation in Pumpâ€“Probe Vibrational Spectroscopy of Hydrogen-Bonded Liquids. Journal of Chemical Theory and Computation, 2017, 13, 1284-1292.	2.3	18
45	A Strategy to Suppress Phonon Transport in Molecular Junctions Using Ï€-Stacked Systems. Journal of Physical Chemistry C, 2017, 121, 7175-7182.	1.5	47
46	Experimental and theoretical evidence for bilayer-by-bilayer surface melting of crystalline ice. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 227-232.	3.3	131
47	Combined Experimental and Theoretical Investigation of Heating Rate on Growth of Iron Oxide Nanoparticles. Chemistry of Materials, 2017, 29, 9648-9656.	3.2	37
48	Bimodal Grain-Size Scaling of Thermal Transport in Polycrystalline Graphene from Large-Scale Molecular Dynamics Simulations. Nano Letters, 2017, 17, 5919-5924.	4.5	28
49	Native surface oxide turns alloyed silicon membranes into nanophononic metamaterials with ultralow thermal conductivity. Physical Review B, 2017, 95, .	1.1	53
50	Dissociative Adsorption of Water at (211) Stepped Metallic Surfaces by First-Principles Simulations. Journal of Physical Chemistry C, 2017, 121, 16783-16791.	1.5	11
51	Thermal conductivity decomposition in two-dimensional materials: Application to graphene. Physical Review B, 2017, 95, .	1.1	113
52	Toward Hamiltonian Adaptive QM/MM: Accurate Solvent Structures Using Many-Body Potentials. Journal of Chemical Theory and Computation, 2016, 12, 3441-3448.	2.3	41
53	Effect of van der Waals interactions on the chemisorption and physisorption of phenol and phenoxy on metal surfaces. Journal of Chemical Physics, 2016, 145, 104701.	1.2	21
54	Optimal thickness of silicon membranes to achieve maximum thermoelectric efficiency: A first principles study. Applied Physics Letters, 2016, 109, 053902.	1.5	13

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55	From Classical to Quantum and Back: A Hamiltonian Scheme for Adaptive Multiresolution Classical/Path-Integral Simulations. Journal of Chemical Theory and Computation, 2016, 12, 3030-3039.	2.3	20
56	Highly anisotropic thermal conductivity of arsenene: Anab initiostudy. Physical Review B, 2016, 93, .	1.1	114
57	Blocking Phonon Transport by Structural Resonances in Alloy-Based Nanophononic Metamaterials Leads to Ultralow Thermal Conductivity. Physical Review Letters, 2016, 117, 025503.	2.9	153
58	Simulation of Dimensionality Effects in Thermal Transport. Lecture Notes in Physics, 2016, , 275-304.	0.3	3
59	Accurate and general treatment of electrostatic interaction in Hamiltonian adaptive resolution simulations. European Physical Journal: Special Topics, 2016, 225, 1505-1526.	1.2	17
60	Microscopic Mechanism and Kinetics of Ice Formation at Complex Interfaces: Zooming in on Kaolinite. Journal of Physical Chemistry Letters, 2016, 7, 2350-2355.	2.1	77
61	Nanophononics: state of the art and perspectives. European Physical Journal B, 2016, 89, 1.	0.6	149
62	Hierarchical thermoelectrics: crystal grain boundaries as scalable phonon scatterers. Nanoscale, 2016, 8, 3729-3738.	2.8	17
63	Adsorption of polyiodobenzene molecules on the Pt(111) surface using van der Waals density functional theory. Surface Science, 2016, 644, 113-121.	0.8	6
64	Molecular Mechanism of Crystal Growth Inhibition at the Calcium Oxalate/Water Interfaces. Journal of Physical Chemistry C, 2016, 120, 4410-4417.	1.5	13
65	Force and heat current formulas for many-body potentials in molecular dynamics simulations with applications to thermal conductivity calculations. Physical Review B, 2015, 92, .	1.1	215
66	Electron-phonon interaction and thermal boundary resistance at the crystal-amorphous interface of the phase change compound GeTe. Journal of Applied Physics, 2015, 117, .	1.1	41
67	Molecular simulation of oligo-glutamates in a calcium-rich aqueous solution: insights into peptide-induced polymorph selection. CrystEngComm, 2015, 17, 6863-6867.	1.3	9
68	Statistical mechanics of Hamiltonian adaptive resolution simulations. Journal of Chemical Physics, 2015, 142, 064115.	1.2	49
69	Freezing point depression in model Lennard-Jones solutions. Molecular Physics, 2015, 113, 2725-2734.	0.8	5
70	Thermal transport in free-standing silicon membranes: influence of dimensional reduction and surface nanostructures. European Physical Journal B, 2015, 88, 1.	0.6	27
71	Tuning Thermal Transport in Ultrathin Silicon Membranes by Surface Nanoscale Engineering. ACS Nano, 2015, 9, 3820-3828.	7.3	104
72	Mechanical Tuning of Thermal Transport in a Molecular Junction. Journal of Physical Chemistry C, 2015, 119, 24636-24642.	1.5	49

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73	Trends in the Adsorption and Dissociation of Water Clusters on Flat and Stepped Metallic Surfaces. Journal of Physical Chemistry C, 2014, 118, 29990-29998.	1.5	27
74	Length-dependent thermal conductivity in suspended single-layer graphene. Nature Communications, 2014, 5, 3689.	5.8	735
75	Hyperbranched Unsaturated Polyphosphates as a Protective Matrix for Long-Term Photon Upconversion in Air. Journal of the American Chemical Society, 2014, 136, 11057-11064.	6.6	109
76	A unified framework for force-based and energy-based adaptive resolution simulations. Europhysics Letters, 2014, 108, 30007.	0.7	29
77	Nuclear Quantum Effects in Water: A Multiscale Study. Journal of Chemical Theory and Computation, 2014, 10, 816-824.	2.3	42
78	Interaction of Charged Amino-Acid Side Chains with Ions: An Optimization Strategy for Classical Force Fields. Journal of Physical Chemistry B, 2014, 118, 3960-3972.	1.2	41
79	Tuning the Adsorption of Aromatic Molecules on Platinum via Halogenation. Journal of Physical Chemistry C, 2014, 118, 6235-6241.	1.5	21
80	Thermal conductivity of one-, two- and three-dimensional sp²carbon. New Journal of Physics, 2013, 15, 105019.	1.2	29
81	Divergence of the thermal conductivity in uniaxially strained graphene. Physical Review B, 2013, 87, .	1.1	131
82	Dimensionality and heat transport in Si-Ge superlattices. Applied Physics Letters, 2013, 102, .	1.5	47
83	Water Release from Pyrophyllite during the Dehydroxylation Process Explored by Quantum Mechanical Simulations. Journal of Physical Chemistry C, 2013, 117, 7526-7532.	1.5	7
84	Particle Formation in the Emulsionâ€Solvent Evaporation Process. Small, 2013, 9, 3514-3522.	5.2	71
85	Hamiltonian Adaptive Resolution Simulation for Molecular Liquids. Physical Review Letters, 2013, 110, 108301.	2.9	145
86	Ice nucleation at the nanoscale probes no manâ€™s land of water. Nature Communications, 2013, 4, 1887.	5.8	112
87	Monte Carlo Adaptive Resolution Simulation of Multicomponent Molecular Liquids. Physical Review Letters, 2013, 111, 060601.	2.9	67
88	Atomistic simulations of heat transport in real-scale silicon nanowire devices. Applied Physics Letters, 2012, 100, .	1.5	12
89	Lattice thermal conductivity of semiconducting bulk materials: atomistic simulations. Physical Chemistry Chemical Physics, 2012, 14, 16209.	1.3	111
90	Adsorption of Dichlorobenzene on Au and Pt Stepped Surfaces Using van der Waals Density Functional Theory. Journal of Physical Chemistry C, 2012, 116, 20409-20416.	1.5	27

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91	Autocatalytic and Cooperatively Stabilized Dissociation of Water on a Stepped Platinum Surface. Journal of the American Chemical Society, 2012, 134, 19217-19222.	6.6	53
92	Thermal transport in phase-change materials from atomistic simulations. Physical Review B, 2012, 86, .	1.1	75
93	Ab initiocharacterization of graphene nanoribbons and their polymer precursors. Journal of Physics Condensed Matter, 2012, 24, 104023.	0.7	3
94	Proton Wires via One-Dimensional Water Chains Adsorbed on Metallic Steps. Journal of Chemical Theory and Computation, 2011, 7, 2681-2684.	2.3	9
95	First Principles Simulations of the Infrared Spectrum of Liquid Water Using Hybrid Density Functionals. Journal of Chemical Theory and Computation, 2011, 7, 1443-1449.	2.3	139
96	Homogeneous ice nucleation from supercooled water. Physical Chemistry Chemical Physics, 2011, 13, 19807.	1.3	226
97	Atomistic calculation of the thermal conductance of large scale bulk-nanowire junctions. Physical Review B, 2011, 84, .	1.1	17
98	Morphology and Temperature Dependence of the Thermal Conductivity of Nanoporous SiGe. Nano Letters, 2011, 11, 3608-3611.	4.5	51
99	Thermal Transport in Nanoporous Silicon: Interplay between Disorder at Mesoscopic and Atomic Scales. ACS Nano, 2011, 5, 1839-1844.	7.3	122
100	Heat transport in amorphous silicon: Interplay between morphology and disorder. Applied Physics Letters, 2011, 98, .	1.5	110
101	Stability of hydrocarbons at deep Earth pressures and temperatures. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 6843-6846.	3.3	72
102	Stability of hydrocarbons at deep Earth pressures and temperatures. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, C168-C168.	0.3	0
103	Silicon stops heat in its tracks. Nature Nanotechnology, 2010, 5, 701-702.	15.6	15
104	Cluster expansion and optimization of thermal conductivity in SiGe nanowires. Physical Review B, 2010, 81, .	1.1	31
105	Ab initioinvestigation of the melting line of nitrogen at high pressure. Physical Review B, 2010, 82, .	1.1	29
106	Exploring the Rehydroxylation Reaction of Pyrophyllite by Ab Initio Molecular Dynamics. Journal of Physical Chemistry B, 2010, 114, 7593-7601.	1.2	17
107	Temperature Dependence of the Thermal Conductivity of Thin Silicon Nanowires. Nano Letters, 2010, 10, 847-851.	4.5	146
108	First-Principle Analysis of the IR Stretching Band of Liquid Water. Journal of Physical Chemistry Letters, 2010, 1, 1398-1402.	2.1	45

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109	Nucleation of tetrahedral solids: A molecular dynamics study of supercooled liquid silicon. Journal of Chemical Physics, 2009, 131, 224519.	1.2	34
110	PLUMED: A portable plugin for free-energy calculations with molecular dynamics. Computer Physics Communications, 2009, 180, 1961-1972.	3.0	1,448
111	Surface-induced crystallization in supercooled tetrahedral liquids. Nature Materials, 2009, 8, 726-730.	13.3	84
112	Theoretical investigation of methane under pressure. Journal of Chemical Physics, 2009, 130, 164520.	1.2	14
113	Atomistic Simulations of Heat Transport in Silicon Nanowires. Physical Review Letters, 2009, 102, 195901.	2.9	251
114	Electronic Effects in the IR Spectrum of Water under Confinement. Journal of Physical Chemistry B, 2009, 113, 4170-4175.	1.2	30
115	Practical algorithms to facilitate large-scale first-principles molecular dynamics. Journal of Physics: Conference Series, 2009, 180, 012074.	0.3	6
116	Pressureâ€induced phase transitions in silicon studied by neural networkâ€based metadynamics simulations. Physica Status Solidi (B): Basic Research, 2008, 245, 2618-2629.	0.7	68
117	Influence of Temperature and Anisotropic Pressure on the Phase Transitions in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-Cristobalite. Physical Review Letters, 2008, 100, 165502.	2.9	38
118	Simulation of the grafting of organosilanes at the surface of dry amorphous silica. Journal of Physics Condensed Matter, 2008, 20, 224011.	0.7	4
119	Probing Properties of Water under Confinement: Infrared Spectra. Nano Letters, 2008, 8, 2959-2962.	4.5	30
120	Metadynamics Simulations of the High-Pressure Phases of Silicon Employing a High-Dimensional Neural Network Potential. Physical Review Letters, 2008, 100, 185501.	2.9	207
121	DFT Research on the Dehydroxylation Reaction of Pyrophyllite 2. Characterization of Reactants, Intermediates, And Transition States along the Reaction Path. Journal of Physical Chemistry A, 2008, 112, 6373-6383.	1.1	17
122	DFT Research on the Dehydroxylation Reaction of Pyrophyllite 1. First-Principle Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2008, 112, 7051-7060.	1.2	43
123	From four- to six-coordinated silica: Transformation pathways from metadynamics. Physical Review B, 2007, 76, .	1.1	45
124	The interplay between surfaceâ€“water and hydrogen bonding in a water adlayer on Pt(111) and Ag(111). Journal of Physics Condensed Matter, 2007, 19, 242101.	0.7	13
125	Thermal Conductivity of Isolated and Interacting Carbon Nanotubes: Comparing Results from Molecular Dynamics and the Boltzmann Transport Equation. Physical Review Letters, 2007, 99, 255502.	2.9	171
126	â€œSite Bindingâ€•of Ca2+Ions to Polyacrylates in Water:Â A Molecular Dynamics Study of Coiling and Aggregation. Macromolecules, 2007, 40, 3437-3442.	2.2	67

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127	Molecular Dynamics Study of the Solvation of Calcium Carbonate in Water. Journal of Physical Chemistry B, 2007, 111, 12219-12227.	1.2	66
128	Migration of positively charged defects in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-quartz. Physical Review B, 2007, 76, .	1.1	13
129	Canonical sampling through velocity rescaling. Journal of Chemical Physics, 2007, 126, 014101.	1.2	11,867
130	Freezing of a Lennard-Jones Fluid: From Nucleation to Spinodal Regime. Physical Review Letters, 2006, 97, 105701.	2.9	227
131	Crystal structure transformations in SiO2 from classical and ab initio metadynamics. Nature Materials, 2006, 5, 623-626.	13.3	198
132	Non-equilibrium dynamics and structure of interfacial ice. Chemical Physics Letters, 2006, 426, 115-119.	1.2	7
133	Evolution of the structure of amorphous ice: From low-density amorphous through high-density amorphous to very high-density amorphous ice. Journal of Chemical Physics, 2005, 122, 134501.	1.2	77
134	Topological Defects and Bulk Melting of Hexagonal Ice. Journal of Physical Chemistry B, 2005, 109, 5421-5424.	1.2	66
135	Ab initiosimulation of photoinduced transformation of small rings in amorphous silica. Physical Review B, 2005, 71, .	1.1	20
136	Evolution of the structure of amorphous ice - from LDA through HDA to VHDA. Acta Crystallographica Section A: Foundations and Advances, 2005, 61, c87-c87.	0.3	0
137	Polyamorphism of Ice at Low Temperatures from Constant-Pressure Simulations. Physical Review Letters, 2004, 92, 225702.	2.9	93
138	Elastic moduli of nanostructured carbon films. Physical Review B, 2004, 70, .	1.1	7
139	Photoelasticity of sodium silicate glass from first principles. Physical Review B, 2004, 70, .	1.1	39
140	Photoelasticity of crystalline and amorphous silica from first principles. Physical Review B, 2003, 68, .	1.1	31
141	Nanofriction Behavior of Cluster-Assembled Carbon Films. Journal of Nanoscience and Nanotechnology, 2002, 2, 637-643.	0.9	5
142	Atomic scale characterization of nanostructured a-C:H films. European Physical Journal B, 2002, 27, 335-340.	0.6	3
143	Nanofriction behavior of cluster-assembled carbon films. Journal of Nanoscience and Nanotechnology, 2002, 2, 637-43.	0.9	1
144	Dehydroxylation and Silanization of the Surfaces of Î²-Cristobalite Silica:Â An ab Initio Simulation. Journal of Physical Chemistry B, 2001, 105, 8007-8013.	1.2	95

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145	Ab InitioSimulations of Photoinduced Interconversions of Oxygen Deficient Centers in Amorphous Silica. Physical Review Letters, 2001, 87, 195504.	2.9	63
146	Simulation of atomic force microscopy of fractal nanostructured carbon films. Europhysics Letters, 2001, 54, 72-76.	0.7	11
147	Covalent Cluster-Assembled Carbon Solids. , 2001, , 89-126.		4
148	Growth of Nanostructured Carbon Films by Cluster Assembly. Physical Review Letters, 1999, 83, 776-779.	2.9	82
149	PbTe/PbSe Thermoelectric Nanocomposites: The Impact of Length Modulations on Lowering Thermal Conductivity. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 0, , .	0.6	2