Riccardo Rurali

List of Publications by Year
in descending order

157	5,636	87888 38	85541 71
papers	citations	h-index	g-index

158	158	158	7190
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A nanomechanical mass sensor with yoctogram resolution. Nature Nanotechnology, 2012, 7, 301-304.	31.5	855
2	Subnanometer Motion of Cargoes Driven by Thermal Gradients Along Carbon Nanotubes. Science, 2008, 320, 775-778.	12.6	322
3	Colloquium: Structural, electronic, and transport properties of silicon nanowires. Reviews of Modern Physics, 2010, 82, 427-449.	45.6	305
4	Fullerene Coalescence in Nanopeapods:â€‰ A Path to Novel Tubular Carbon. Nano Letters, 2003, 3, 1037-1042.	9.1	185
5	Metallic and Semimetallic SiliconâŸ¨100âŸ©Nanowires. Physical Review Letters, 2005, 94, 026805.	7.8	164
6	Polarity Assignment in ZnTe, GaAs, ZnO, and GaN-AlN Nanowires from Direct Dumbbell Analysis. Nano Letters, 2012, 12, 2579-2586.	9.1	161
7	Quantum-size effects in hafnium-oxide resistive switching. Applied Physics Letters, 2013, 102, 183505.	3.3	151
8	Siliconâ€“Germanium Nanowires: Chemistry and Physics in Play, from Basic Principles to Advanced Applications. Chemical Reviews, 2014, 114, 1371-1412.	47.7	151
9	Electronic Transport between Graphene Layers Covalently Connected by Carbon Nanotubes. ACS Nano, 2010, 4, 7596-7602.	14.6	133
10	Scaling Theory Put into Practice: First-Principles Modeling of Transport in Doped Silicon Nanowires. Physical Review Letters, 2007, 99, 076803.	7.8	112
11	Electronic transport through Si nanowires: Role of bulk and surface disorder. Physical Review B, 2006, 74, .	3.2	95
12	Prediction of Ordered Phases of Encapsulated C60, C70, and C78Inside Carbon Nanotubes. Nano Letters, 2005, 5, 349-355.	9.1	85
13	Trocadero: a multiple-algorithm multiple-model atomistic simulation program. Computational Materials Science, 2003, 28, 85-106.	3.0	75
14	Transport properties of oxygen vacancy filaments in metal/crystalline or amorphous HfO<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>/metal structures. Physical Review B, 2012, 86, .	3.2	70
15	Comment on â€œMolecular Distortions and Chemical Bonding of a Largeï€-Conjugated Molecule on a Metal Surfaceâ€• Physical Review Letters, 2005, 95, 209601; author reply 209602.	7.8	68
16	Thermal Rectification by Design in Telescopic Si Nanowires. Nano Letters, 2015, 15, 8255-8259.	9.1	66
17	Electronic and structural properties of silicon carbide nanowires. Physical Review B, 2005, 71, .	3.2	63
18	Prediction of giant electroactuation for papyruslike carbon nanoscroll structures: First-principles calculations. Physical Review B, 2006, 74, .	3.2	63

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19	Molecular orbital shift of perylenetetracarboxylic-dianhydride on gold. Chemical Physics Letters, 2007, 438, 249-253.	2.6	63
20	Band-Offset Driven Efficiency of the Doping of SiGe Coreâ"Shell Nanowires. Nano Letters, 2011, 11, 594-598.	9.1	63
21	A review on IIIâ€"V coreâ€"multishell nanowires: growth, properties, and applications. Journal Physics D: Applied Physics, 2017, 50, 143001.	2.8	63
22	Single-molecule manipulation and chemistry with the STM. Journal of Physics Condensed Matter, 2005, 17, S1049-S1074.	1.8	62
23	Theory of Defects in One-Dimensional Systems: Application to Al-Catalyzed Si Nanowires. Nano Letters, 2009, 9, 975-979.	9.1	62
24	Charge corrections for supercell calculations of defects in semiconductors. Physica B: Condensed Matter, 2003, 340-342, 190-194.	2.7	60
25	Multi-scale quantum point contact model for filamentary conduction in resistive random access memories devices. Journal of Applied Physics, 2014, 115, .	2.5	54
26	Trans to cis isomerization of an azobenzene derivative onÂaÂCu(100) surface. Applied Physics A: Materials Science and Processing, 2008, 93, 241-246.	2.3	53
27	Synthesis of PbI₂ Singleâ€Łayered Inorganic Nanotubes Encapsulated Within Carbon Nanotubes. Advanced Materials, 2014, 26, 2016-2021.	21.0	52
28	Heat transport across a SiGe nanowire axial junction: Interface thermal resistance and thermal rectification. Physical Review B, 2014, 90, .	3.2	51
29	Optical Emission in Hexagonal SiGe Nanowires. Nano Letters, 2017, 17, 4753-4758.	9.1	51
30	Electron Transport via Local Polarons at Interface Atoms. Physical Review Letters, 2006, 97, 206801.	7.8	50
31	Site-Dependent Coordination Bonding in Self-Assembled Metalâ"Organic Networks. Journal of Physical Chemistry Letters, 2011, 2, 55-61.	4.6	46
32	Model for thermal conductivity in nanoporous silicon from atomistic simulations. Physical Review B, 2015, 91, .	3.2	46
33	Ferrodistortive Instability at the (001) Surface of Half-Metallic Manganites. Physical Review Letters, 2007, 99, 226101.	7.8	40
34	Observation of second sound in a rapidly varying temperature field in Ge. Science Advances, 2021, 7, .	10.3	40
35	Accurate single-particle determination of the band gap in silicon nanowires. Physical Review B, 2007, 76, .	3.2	39
36	Molecular Doping and Subsurface Dopant Reactivation in Si Nanowires. Nano Letters, 2010, 10, 3590-3595.	9.1	39

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37	Band gap engineering of MoS2 upon compression. Journal of Applied Physics, 2016, 119, .	2.5	39
38	A phononic switch based on ferroelectric domain walls. Physical Review B, 2017, 96, .	3.2	39
39	Thermal conductivity and phonon hydrodynamics in transition metal dichalcogenides from first-principles. 2D Materials, 2019, 6, 035002.	4.4	39
40	Crystal Phase Effects in Si Nanowire Polytypes and Their Homojunctions. Nano Letters, 2016, 16, 5694-5700.	9.1	38
41	Size effects in surface-reconstructedâŸ¨100âŸ©andâŸ¨110âŸ©silicon nanowires. Physical Review B, 2006, 74, .	3.2	37
42	Surface physics of semiconducting nanowires. Progress in Surface Science, 2016, 91, 1-28.	8.3	36
43	Modeling Transport in Ultrathin Si Nanowires: Charged versus Neutral Impurities. Nano Letters, 2008, 8, 2825-2828.	9.1	34
44	Thermally induced directed motion of fullerene clusters encapsulated in carbon nanotubes. Chemical Physics Letters, 2010, 497, 62-65.	2.6	33
45	On the properties of surface reconstructed silicon nanowires. Nanotechnology, 2005, 16, S250-S253.	2.6	32
46	Crystalline, Phononic, and Electronic Properties of Heterostructured Polytypic Ge Nanowires by Raman Spectroscopy. Nano Letters, 2018, 18, 7075-7084.	9.1	32
47	Phonon Engineering in Twinning Superlattice Nanowires. Nano Letters, 2019, 19, 4702-4711.	9.1	31
48	Piezoelectric monolayers as nonlinear energy harvesters. Nanotechnology, 2014, 25, 175401.	2.6	30
49	Thermal rectification in silicon by a graded distribution of defects. Journal of Applied Physics, 2016, 119, .	2.5	30
50	Convergence study of neutral and charged defect formation energies in Si nanowires. Physical Review B, 2010, 81, .	3.2	29
51	Donor levels in Si nanowires determined by hybrid-functional calculations. Physical Review B, 2009, 79, .	3.2	28
52	Nanostructured graphene for energy harvesting. Physical Review B, 2011, 84, .	3.2	27
53	Ferroelectric domain wall phonon polarizer. Physical Review Materials, 2017, 1, .	2.4	27
54	Theoretical evidence for the kick-out mechanism for B diffusion in SiC. Applied Physics Letters, 2002, 81, 2989-2991.	3.3	26

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55	Noise energy harvesting in buckled BN nanoribbons from molecular dynamics. Nano Energy, 2015, 15, 329-334.	16.0	25
56	Heat transport through a solidâ€“solid junction: the interface as an autonomous thermodynamic system. Physical Chemistry Chemical Physics, 2016, 18, 13741-13745.	2.8	25
57	Electric control of the heat flux through electrophononic effects. Physical Review B, 2018, 97, .	3.2	25
58	First-principles study of n-type dopants and their clustering in SiC. Applied Physics Letters, 2003, 82, 4298-4300.	3.3	24
59	First-principles studies of the diffusion of B impurities and vacancies in SiC. Physical Review B, 2004, 69, .	3.2	24
60	NH3 molecular doping of silicon nanowires grown along the [112], [110], [001], and [111] orientations. Nanoscale Research Letters, 2012, 7, 308.	5.7	24
61	Thermal transport in porous Si nanowires from approach-to-equilibrium molecular dynamics calculations. Applied Physics Letters, 2016, 109, .	3.3	24
62	Interaction of Boron and Phosphorus Impurities in Silicon Nanowires during Low-Temperature Ozone Oxidation. Journal of Physical Chemistry C, 2013, 117, 20300-20307.	3.1	22
63	Thermal conductivity of hexagonal Si and hexagonal Si nanowires from first-principles. Applied Physics Letters, 2017, 111, .	3.3	21
64	Structured Graphene Devices for Mass Transport. Small, 2011, 7, 775-780.	10.0	20
65	Electron Transport in SiGe Alloy Nanowires in the Ballistic Regime from First-Principles. Nano Letters, 2012, 12, 2717-2721.	9.1	20
66	Thermal boundary resistance from transient nanocalorimetry: A multiscale modeling approach. Physical Review B, 2017, 95, .	3.2	20
67	Reversible scaling simulations of the melting transition in silicon. Physical Review B, 2004, 69, .	3.2	19
68	An experimental test on the distribution of positronium lifetimes in polymers. Chemical Physics, 1998, 237, 493-499.	1.9	18
69	First principles studies of neutral vacancies diffusion in SiC. Computational Materials Science, 2003, 27, 36-42.	3.0	18
70	Room Temperature Observation of Quantum Confinement in Single InAs Nanowires. Nano Letters, 2015, 15, 481-485.	9.1	18
71	Molecules on vicinal Au surfaces studied by scanning tunnelling microscopy. Journal of Physics Condensed Matter, 2006, 18, S51-S66.	1.8	17
72	Phonon transport across crystal-phase interfaces and twin boundaries in semiconducting nanowires. Nanoscale, 2019, 11, 16007-16016.	5.6	17

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73	Probing Lattice Dynamics and Electronic Resonances in Hexagonal Ge and Si_xGe_{1â€“x} Alloys in Nanowires by Raman Spectroscopy. ACS Nano, 2020, 14, 6845-6856.	14.6	17
74	Atypical charge redistribution over a charge-transfer monolayer on a metal. New Journal of Physics, 2013, 15, 083048.	2.9	16
75	Impact of pore anisotropy on the thermal conductivity of porous Si nanowires. Scientific Reports, 2018, 8, 12796.	3.3	16
76	Structural and electronic properties of zigzag carbon nanotubes filled with small fullerenes. Journal of Physics Condensed Matter, 2007, 19, 236222.	1.8	15
77	Transport in silicon nanowires: role of radial dopant profile. Journal of Computational Electronics, 2008, 7, 324-327.	2.5	15
78	C60adsorption on theSi(111)-p(7Ã—7)surface: A theoretical study. Physical Review B, 2010, 81, .	3.2	15
79	Tuning thermal transport in Si nanowires by isotope engineering. Physical Chemistry Chemical Physics, 2016, 18, 26262-26267.	2.8	15
80	Mn-doped silicon nanowires: First-principles calculations. Physical Review B, 2008, 78, .	3.2	14
81	Using high pressure to unravel the mechanism of visible emission in amorphous Si/SiOxnanoparticles. Physical Review B, 2014, 89, .	3.2	14
82	Shell-Thickness Controlled Semiconductorâ€“Metal Transition in Siâ€“SiC Coreâ€“Shell Nanowires. Nano Letters, 2015, 15, 3425-3430.	9.1	14
83	Thermal conductivity for III-V and II-VI semiconductor wurtzite and zinc-blende polytypes: The role of anharmonicity and phase space. Physical Review Materials, 2019, 3, .	2.4	14
84	Inducing bistability with local electret technology in a microcantilever based non-linear vibration energy harvester. Applied Physics Letters, 2013, 102, .	3.3	13
85	Fabrication of highly regular suspended graphene nanoribbons through a one-step electron beam lithography process. Microelectronic Engineering, 2014, 129, 81-85.	2.4	13
86	Electron and phonon transport in twisted graphene nanoribbons. Journal Physics D: Applied Physics, 2017, 50, 234005.	2.8	13
87	Thermal conductivity changes across a structural phase transition: The case of high-pressure silica. Physical Review B, 2017, 96, .	3.2	13
88	Strain engineering of ZnO thermal conductivity. Physical Review Materials, 2019, 3, .	2.4	13
89	Giant Thermal Transport Tuning at a Metal/Ferroelectric Interface. Advanced Materials, 2022, 34, e2105778.	21.0	13
90	Giant Electrophononic Response in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>PbTiO</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow> by Strain Engineering. Physical Review Letters, 2019, 123, 185901.	7.8	12

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91	Highly Biaxially Strained Silicene on Au(111). Journal of Physical Chemistry C, 2021, 125, 9973-9980.	3.1	12
92	Theoretical investigation of lattice thermal conductivity and electrophononic effects in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></m Physical Review Materials, 2019, 3, .	2.4	12
93	Transition metal-decorated germanene for NO, N2 and O2 sensing: A DFT study. Surfaces and Interfaces, 2022, 30, 101886.	3.0	12
94	Interconnection effects on the electronic and optical properties of Ge nanostructures: A semi-empirical approach. Physica E: Low-Dimensional Systems and Nanostructures, 2012, 44, 1230-1235.	2.7	11
95	Optical absorption modulation by selective codoping of SiGe core-shell nanowires. Journal of Applied Physics, 2012, 112, .	2.5	11
96	Structural and electronic properties of Si1â^'xGex alloy nanowires. Journal of Applied Physics, 2014, 116, 154301.	2.5	11
97	Thermal Conductivity of Rutile and Anatase TiO2 from First-Principles. Journal of Physical Chemistry C, 2019, 123, 30851-30855.	3.1	11
98	Experimental demonstration of the suppression of optical phonon splitting in 2D materials by Raman spectroscopy. 2D Materials, 2020, 7, 035017.	4.4	11
99	Spontaneous Formation of Triptycene Supramolecules on Surfaces. Journal of Physical Chemistry B, 2006, 110, 20089-20092.	2.6	10
100	Spin transport in dangling-bond wires on doped H-passivated Si(100). Nanotechnology, 2014, 25, 465703.	2.6	10
101	Preferential Positioning, Stability, and Segregation of Dopants in Hexagonal Si Nanowires. Nano Letters, 2019, 19, 866-876.	9.1	10
102	New insights in the lattice dynamics of monolayers, bilayers, and trilayers of WSe₂ and unambiguous determination of few-layer-flakesâ€™ thickness. 2D Materials, 2020, 7, 025004.	4.4	10
103	First stages of the oxidation of the Si-rich 3Câ€“SiC(001) surface. Computational Materials Science, 2005, 33, 13-19.	3.0	9
104	Band bending and quasiâ€2DEG in the metallized Î²â€6SiC(001) surface. Physica Status Solidi - Rapid Research Letters, 2008, 2, 218-220.	2.4	9
105	Scattering cross section of metal catalyst atoms in silicon nanowires. Physical Review B, 2010, 81, .	3.2	9
106	Thermal boundary resistance in semiconductors by non-equilibrium thermodynamics. Advances in Physics: X, 2016, 1, 246-261.	4.1	9
107	Manipulating phonons at the nanoscale: Impurities and boundaries. Current Opinion in Green and Sustainable Chemistry, 2019, 17, 1-7.	5.9	9
108	Ordered arrays of quantum wires through hole patterning: ab initio and empirical electronic structure calculations. Applied Physics Letters, 2007, 90, 083118.	3.3	8

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109	Doping of SiGe core-shell nanowires. Journal of Computational Electronics, 2012, 11, 272-279.	2.5	8
110	Molecular doping and gas sensing in Si nanowires: From charge injection to reduced dielectric mismatch. Journal of Applied Physics, 2013, 114, 204302.	2.5	8
111	Anisotropy-driven thermal conductivity switching and thermal hysteresis in a ferroelectric. Applied Physics Letters, 2019, 115, 192903.	3.3	8
112	Anisotropic Thermal Conductivity in Few-Layer and Bulk Titanium Trisulphide from First Principles. Nanomaterials, 2020, 10, 704.	4.1	8
113	Unveiling Planar Defects in Hexagonal Group IV Materials. Nano Letters, 2021, 21, 3619-3625.	9.1	8
114	Optimisation of the thermoelectric efficiency of zirconium trisulphide monolayers through unixial and biaxial strain. Nanoscale Advances, 2020, 2, 5352-5361.	4.6	8
115	Understanding doping at the nanoscale: the case of codoped Si and Ge nanowires. Journal Physics D: Applied Physics, 2014, 47, 394013.	2.8	7
116	Interface driven thermal rectification in a grapheneâ€“bilayer graphene junction from nonequilibrium molecular dynamics. Journal of Applied Physics, 2018, 124, .	2.5	7
117	Indications of Phonon Hydrodynamics in Telescopic Silicon Nanowires. Physical Review Applied, 2019, 11, .	3.8	7
118	Dynamical tuning of the thermal conductivity via magnetophononic effects. Physical Review B, 2022, 105, .	3.2	7
119	The BN-pair impurity in carbon nanotubes and the possibility for disorder-induced frustration of gap formation. Nanotechnology, 2008, 19, 445709.	2.6	6
120	Ab Initio Study of Phosphorus Donors Acting as Quantum Bits in Silicon Nanowires. Nano Letters, 2012, 12, 3460-3465.	9.1	6
121	Buckling suspended graphene nanoribbons to harvest energy from noisy vibrations. Microelectronic Engineering, 2013, 111, 122-125.	2.4	6
122	Conductance fluctuations in Si nanowires studied from first-principles. Journal of Applied Physics, 2014, 116, 074303.	2.5	6
123	Quasiballistic phonon transport from first principles. Physical Review B, 2020, 102, .	3.2	6
124	Strain engineering of the electronic and thermoelectric properties of titanium trisulphide monolayers. Nano Express, 2020, 1, 010026.	2.4	6
125	Interface-driven thermal rectification in nanoscale systems. Physical Review Materials, 2018, 2, .	2.4	6
126	A Thermal Switch for Coherent Phonons Based on a Molecular Junction. Journal of Physical Chemistry C, 2017, 121, 10571-10576.	3.1	5

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127	Ab initio studies of the optoelectronic structure of undoped and doped silicon nanocrystals and nanowires: the role of size, passivation, symmetry and phase. Faraday Discussions, 2020, 222, 217-239.	3.2	5
128	Silicon nanowires as acetone-adsorptive media for diabetes diagnosis. Applied Surface Science, 2021, 547, 149175.	6.1	5
129	Large electromechanical response in silicon nanowires predicted from first-principles electronic structure calculations. Physical Review B, 2008, 77, .	3.2	4
130	First-principles calculations of SO2 sensing with Si nanowires. European Physical Journal B, 2016, 89, 1.	1.5	4
131	Doping of IIIâ€“V Arsenide and Phosphide Wurtzite Semiconductors. Journal of Physical Chemistry C, 2020, 124, 27203-27212.	3.1	4
132	First-Principles Study of O Adsorption at SiC Surface. Materials Science Forum, 2004, 457-460, 1293-1296.	0.3	3
133	Nonlinear dynamics in a graphene nanostructured device for energy harvesting. , 2013, , .		3
134	First-Principles Studies of N and P Dopant Interactions in SiC: Implications for Co-Doping. Materials Science Forum, 2003, 433-436, 649-652.	0.3	2
135	The thermal boundary resistance at semiconductor interfaces: a critical appraisal of the Onsager vs. Kapitza formalisms. Physical Chemistry Chemical Physics, 2018, 20, 22623-22628.	2.8	2
136	Low-temperature thermal rectification by tailoring isotope distributions. Physical Review B, 2019, 99, .	3.2	2
137	Interatomic potential for predicting the thermal conductivity of zirconium trisulfide monolayers with molecular dynamics. Journal of Applied Physics, 2021, 129, .	2.5	2
138	Gas and Liquid Doping Gas and liquid doping of Porous Silicon. , 2014, , 639-645.		2
139	Ab Initio Calculations of B Diffusion in SiC. Materials Science Forum, 2002, 389-393, 553-556.	0.3	1
140	Self-passivation mechanisms in clusters of N dopants in SiC. Physica Status Solidi C: Current Topics in Solid State Physics, 2004, 1, 274-277.	0.8	1
141	Fabrication of ordered arrays of quantum wires through hole patterning. Journal of Physics: Conference Series, 2008, 100, 052049.	0.4	1
142	Pattern transfer optimization for the fabrication of arrays of silicon nanowires. Microelectronic Engineering, 2010, 87, 1479-1482.	2.4	1
143	PtSi Clustering in Silicon Probed by Transport Spectroscopy. Physical Review X, 2013, 3, .	8.9	1
144	Carbon Nanotubes: Synthesis of PbI2Single-Layered Inorganic Nanotubes Encapsulated Within Carbon Nanotubes (Adv. Mater. 13/2014). Advanced Materials, 2014, 26, 2108-2108.	21.0	1

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145	Special issue on thermoelectric properties of nanostructured materials. Journal Physics D: Applied Physics, 2018, 51, 430301.	2.8	1
146	Tunable thermal conductivity of ternary alloy semiconductors from first-principles. Journal Physics D: Applied Physics, 2021, 54, 335302.	2.8	1
147	Nonlinear Dynamics of an Ambient Noise Driven Array of Coupled Graphene Nanostructured Devices for Energy Harvesting. MATEC Web of Conferences, 2014, 16, 01001.	0.2	1
148	Defect dynamics in P+ implanted 6H -SiC studied by positron annihilation spectroscopy. Physica Status Solidi C: Current Topics in Solid State Physics, 2004, 1, 257-260.	0.8	0
149	Graphene Devices: Structured Graphene Devices for Mass Transport (Small 6/2011). Small, 2011, 7, 698-698.	10.0	0
150	Electrical evidence of atomic-size effects in the conduction filament of RRAM. , 2012, , .		0
151	Piezoelectric 2D materials for bistable NEMS energy harvesters. Materials Research Society Symposia Proceedings, 2014, 1701, 1.	0.1	0
152	Gas and Liquid Doping of Porous Silicon. , 2014, , 1-7.		0
153	Thermal rectification. , 2018, , .		0
154	SiGe Nanowires for Thermoelectrics Applications. Lecture Notes in Nanoscale Science and Technology, 2014, , 497-515.	0.8	0
155	Gas and Liquid Doping of Porous Silicon. , 2018, , 973-979.		0
156	Using Thermal Gradients for Actuation in the Nanoscale. IUTAM Symposium on Cellular, Molecular and Tissue Mechanics, 2009, , 141-150.	0.2	0
157	Theoretical Aspects of Point Defects inÂSemiconductor Nanowires. , 2021, , 349-367.		0