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	Giant Thermal Transport Tuning at a Metal/Ferroelectric Interface. Advanced Materials, 2022, 34, e2105778.	21.0	13
2	Dynamical tuning of the thermal conductivity via magnetophononic effects. Physical Review B, 2022, 105, .	3.2	7
3	Transition metal-decorated germanene for NO, N2 and O2 sensing: A DFT study. Surfaces and Interfaces, 2022, 30, 101886.	3.0	12
4	Interatomic potential for predicting the thermal conductivity of zirconium trisulfide monolayers with molecular dynamics. Journal of Applied Physics, 2021, 129, .	2.5	2
5	Unveiling Planar Defects in Hexagonal Group IV Materials. Nano Letters, 2021, 21, 3619-3625.	9.1	8
6	Highly Biaxially Strained Silicene on Au(111). Journal of Physical Chemistry C, 2021, 125, 9973-9980.	3.1	12
7	Silicon nanowires as acetone-adsorptive media for diabetes diagnosis. Applied Surface Science, 2021, 547, 149175.	6.1	5
8	Tunable thermal conductivity of ternary alloy semiconductors from first-principles. Journal Physics D: Applied Physics, 2021, 54, 335302.	2.8	1
9	Observation of second sound in a rapidly varying temperature field in Ge. Science Advances, 2021, 7, .	10.3	40
10	Theoretical Aspects of Point Defects inÂSemiconductor Nanowires. , 2021, , 349-367.		0
11	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
12	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
13	Quasiballistic phonon transport from first principles. Physical Review B, 2020, 102, .	3.2	6
14	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
15	Experimental demonstration of the suppression of optical phonon splitting in 2D materials by Raman spectroscopy. 2D Materials, 2020, 7, 035017.	4.4	11
16	Anisotropic Thermal Conductivity in Few-Layer and Bulk Titanium Trisulphide from First Principles. Nanomaterials, 2020, 10, 704.	4.1	8
17	Strain engineering of the electronic and thermoelectric properties of titanium trisulphide monolayers. Nano Express, 2020, 1, 010026.	2.4	6
18	Doping of IIIâ€“V Arsenide and Phosphide Wurtzite Semiconductors. Journal of Physical Chemistry C, 2020, 124, 27203-27212.	3.1	4

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19	Optimisation of the thermoelectric efficiency of zirconium trisulphide monolayers through unixial and biaxial strain. Nanoscale Advances, 2020, 2, 5352-5361.	4.6	8
20	Phonon transport across crystal-phase interfaces and twin boundaries in semiconducting nanowires. Nanoscale, 2019, 11, 16007-16016.	5.6	17
21	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> by Strain Engineering. Physical Review Letters, 2019, 123, 185901.	7.8	12
22	Phonon Engineering in Twinning Superlattice Nanowires. Nano Letters, 2019, 19, 4702-4711.	9.1	31
23	Indications of Phonon Hydrodynamics in Telescopic Silicon Nanowires. Physical Review Applied, 2019, 11, .	3.8	7
24	Thermal conductivity and phonon hydrodynamics in transition metal dichalcogenides from first-principles. 2D Materials, 2019, 6, 035002.	4.4	39
25	Anisotropy-driven thermal conductivity switching and thermal hysteresis in a ferroelectric. Applied Physics Letters, 2019, 115, 192903.	3.3	8
26	Thermal Conductivity of Rutile and Anatase TiO2 from First-Principles. Journal of Physical Chemistry C, 2019, 123, 30851-30855.	3.1	11
27	Manipulating phonons at the nanoscale: Impurities and boundaries. Current Opinion in Green and Sustainable Chemistry, 2019, 17, 1-7.	5.9	9
28	Preferential Positioning, Stability, and Segregation of Dopants in Hexagonal Si Nanowires. Nano Letters, 2019, 19, 866-876.	9.1	10
29	Low-temperature thermal rectification by tailoring isotope distributions. Physical Review B, 2019, 99, .	3.2	2
30	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> Physical Review Materials, 2019, 3, .	2.4	12
31	Strain engineering of ZnO thermal conductivity. Physical Review Materials, 2019, 3, .	2.4	13
32	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
33	Thermal rectification. , 2018, , .		0
34	Interface driven thermal rectification in a grapheneâ€“bilayer graphene junction from nonequilibrium molecular dynamics. Journal of Applied Physics, 2018, 124, .	2.5	7
35	Special issue on thermoelectric properties of nanostructured materials. Journal Physics D: Applied Physics, 2018, 51, 430301.	2.8	1
36	Crystalline, Phononic, and Electronic Properties of Heterostructured Polytypic Ge Nanowires by Raman Spectroscopy. Nano Letters, 2018, 18, 7075-7084.	9.1	32

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37	Electric control of the heat flux through electrophononic effects. Physical Review B, 2018, 97, .	3.2	25
38	Impact of pore anisotropy on the thermal conductivity of porous Si nanowires. Scientific Reports, 2018, 8, 12796.	3.3	16
39	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
40	Interface-driven thermal rectification in nanoscale systems. Physical Review Materials, 2018, 2, .	2.4	6
41	Gas and Liquid Doping of Porous Silicon. , 2018, , 973-979.		0
42	Thermal boundary resistance from transient nanocalorimetry: A multiscale modeling approach. Physical Review B, 2017, 95, .	3.2	20
43	A review on IIIâ€“V coreâ€“multishell nanowires: growth, properties, and applications. Journal Physics D: Applied Physics, 2017, 50, 143001.	2.8	63
44	A Thermal Switch for Coherent Phonons Based on a Molecular Junction. Journal of Physical Chemistry C, 2017, 121, 10571-10576.	3.1	5
45	Electron and phonon transport in twisted graphene nanoribbons. Journal Physics D: Applied Physics, 2017, 50, 234005.	2.8	13
46	Thermal conductivity of hexagonal Si and hexagonal Si nanowires from first-principles. Applied Physics Letters, 2017, 111, .	3.3	21
47	Thermal conductivity changes across a structural phase transition: The case of high-pressure silica. Physical Review B, 2017, 96, .	3.2	13
48	A phononic switch based on ferroelectric domain walls. Physical Review B, 2017, 96, .	3.2	39
49	Optical Emission in Hexagonal SiGe Nanowires. Nano Letters, 2017, 17, 4753-4758.	9.1	51
50	Ferroelectric domain wall phonon polarizer. Physical Review Materials, 2017, 1, .	2.4	27
51	Thermal transport in porous Si nanowires from approach-to-equilibrium molecular dynamics calculations. Applied Physics Letters, 2016, 109, .	3.3	24
52	First-principles calculations of SO2 sensing with Si nanowires. European Physical Journal B, 2016, 89, 1.	1.5	4
53	Band gap engineering of MoS2 upon compression. Journal of Applied Physics, 2016, 119, .	2.5	39
54	Thermal boundary resistance in semiconductors by non-equilibrium thermodynamics. Advances in Physics: X, 2016, 1, 246-261.	4.1	9

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55	Tuning thermal transport in Si nanowires by isotope engineering. Physical Chemistry Chemical Physics, 2016, 18, 26262-26267.	2.8	15
56	Crystal Phase Effects in Si Nanowire Polytypes and Their Homojunctions. Nano Letters, 2016, 16, 5694-5700.	9.1	38
57	Thermal rectification in silicon by a graded distribution of defects. Journal of Applied Physics, 2016, 119, .	2.5	30
58	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
59	Surface physics of semiconducting nanowires. Progress in Surface Science, 2016, 91, 1-28.	8.3	36
60	Noise energy harvesting in buckled BN nanoribbons from molecular dynamics. Nano Energy, 2015, 15, 329-334.	16.0	25
61	Shell-Thickness Controlled Semiconductorâ€“Metal Transition in Siâ€“SiC Coreâ€“Shell Nanowires. Nano Letters, 2015, 15, 3425-3430.	9.1	14
62	Model for thermal conductivity in nanoporous silicon from atomistic simulations. Physical Review B, 2015, 91, .	3.2	46
63	Thermal Rectification by Design in Telescopic Si Nanowires. Nano Letters, 2015, 15, 8255-8259.	9.1	66
64	Room Temperature Observation of Quantum Confinement in Single InAs Nanowires. Nano Letters, 2015, 15, 481-485.	9.1	18
65	Piezoelectric monolayers as nonlinear energy harvesters. Nanotechnology, 2014, 25, 175401.	2.6	30
66	Spin transport in dangling-bond wires on doped H-passivated Si(100). Nanotechnology, 2014, 25, 465703.	2.6	10
67	Understanding doping at the nanoscale: the case of codoped Si and Ge nanowires. Journal Physics D: Applied Physics, 2014, 47, 394013.	2.8	7
68	Conductance fluctuations in Si nanowires studied from first-principles. Journal of Applied Physics, 2014, 116, 074303.	2.5	6
69	Heat transport across a SiGe nanowire axial junction: Interface thermal resistance and thermal rectification. Physical Review B, 2014, 90, .	3.2	51
70	Piezoelectric 2D materials for bistable NEMS energy harvesters. Materials Research Society Symposia Proceedings, 2014, 1701, 1.	0.1	0
71	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
72	Synthesis of PbI₂ Singleâ€Layered Inorganic Nanotubes Encapsulated Within Carbon Nanotubes. Advanced Materials, 2014, 26, 2016-2021.	21.0	52

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73	Siliconâ€“Germanium Nanowires: Chemistry and Physics in Play, from Basic Principles to Advanced Applications. Chemical Reviews, 2014, 114, 1371-1412.	47.7	151
74	Structural and electronic properties of Si1â^'xGex alloy nanowires. Journal of Applied Physics, 2014, 116, 154301.	2.5	11
75	Gas and Liquid Doping of Porous Silicon. , 2014, , 1-7.		0
76	Multi-scale quantum point contact model for filamentary conduction in resistive random access memories devices. Journal of Applied Physics, 2014, 115, .	2.5	54
77	Fabrication of highly regular suspended graphene nanoribbons through a one-step electron beam lithography process. Microelectronic Engineering, 2014, 129, 81-85.	2.4	13
78	Using high pressure to unravel the mechanism of visible emission in amorphous Si/SiOxnanoparticles. Physical Review B, 2014, 89, .	3.2	14
79	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
80	SiGe Nanowires for Thermoelectrics Applications. Lecture Notes in Nanoscale Science and Technology, 2014, , 497-515.	0.8	0
81	Gas and Liquid Doping Gas and liquid doping of Porous Silicon. , 2014, , 639-645.		2
82	Inducing bistability with local electret technology in a microcantilever based non-linear vibration energy harvester. Applied Physics Letters, 2013, 102, .	3.3	13
83	Buckling suspended graphene nanoribbons to harvest energy from noisy vibrations. Microelectronic Engineering, 2013, 111, 122-125.	2.4	6
84	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
85	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
86	Atypical charge redistribution over a charge-transfer monolayer on a metal. New Journal of Physics, 2013, 15, 083048.	2.9	16
87	Nonlinear dynamics in a graphene nanostructured device for energy harvesting. , 2013, , .		3
88	PtSi Clustering in Silicon Probed by Transport Spectroscopy. Physical Review X, 2013, 3, .	8.9	1
89	Quantum-size effects in hafnium-oxide resistive switching. Applied Physics Letters, 2013, 102, 183505.	3.3	151
90	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

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91	Electrical evidence of atomic-size effects in the conduction filament of RRAM. , 2012, , .		0
92	Polarity Assignment in ZnTe, GaAs, ZnO, and GaN-AlN Nanowires from Direct Dumbbell Analysis. Nano Letters, 2012, 12, 2579-2586.	9.1	161
93	Electron Transport in SiGe Alloy Nanowires in the Ballistic Regime from First-Principles. Nano Letters, 2012, 12, 2717-2721.	9.1	20
94	Doping of SiGe core-shell nanowires. Journal of Computational Electronics, 2012, 11, 272-279.	2.5	8
95	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
96	Ab Initio Study of Phosphorus Donors Acting as Quantum Bits in Silicon Nanowires. Nano Letters, 2012, 12, 3460-3465.	9.1	6
97	NH3 molecular doping of silicon nanowires grown along the [112], [110], [001], and [111] orientations. Nanoscale Research Letters, 2012, 7, 308.	5.7	24
98	Optical absorption modulation by selective codoping of SiGe core-shell nanowires. Journal of Applied Physics, 2012, 112, .	2.5	11
99	A nanomechanical mass sensor with yoctogram resolution. Nature Nanotechnology, 2012, 7, 301-304.	31.5	855
100	Site-Dependent Coordination Bonding in Self-Assembled Metalâ^'Organic Networks. Journal of Physical Chemistry Letters, 2011, 2, 55-61.	4.6	46
101	Nanostructured graphene for energy harvesting. Physical Review B, 2011, 84, .	3.2	27
102	Band-Offset Driven Efficiency of the Doping of SiGe Coreâ^'Shell Nanowires. Nano Letters, 2011, 11, 594-598.	9.1	63
103	Structured Graphene Devices for Mass Transport. Small, 2011, 7, 775-780.	10.0	20
104	Graphene Devices: Structured Graphene Devices for Mass Transport (Small 6/2011). Small, 2011, 7, 698-698.	10.0	0
105	Pattern transfer optimization for the fabrication of arrays of silicon nanowires. Microelectronic Engineering, 2010, 87, 1479-1482.	2.4	1
106	Thermally induced directed motion of fullerene clusters encapsulated in carbon nanotubes. Chemical Physics Letters, 2010, 497, 62-65.	2.6	33
107	Scattering cross section of metal catalyst atoms in silicon nanowires. Physical Review B, 2010, 81, .	3.2	9
108	C60adsorption on theSi(111)-p(7Ã—7)surface: A theoretical study. Physical Review B, 2010, 81, .	3.2	15

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109	Convergence study of neutral and charged defect formation energies in Si nanowires. Physical Review B, 2010, 81, .	3.2	29
110	Colloquium: Structural, electronic, and transport properties of silicon nanowires. Reviews of Modern Physics, 2010, 82, 427-449.	45.6	305
111	Molecular Doping and Subsurface Dopant Reactivation in Si Nanowires. Nano Letters, 2010, 10, 3590-3595.	9.1	39
112	Electronic Transport between Graphene Layers Covalently Connected by Carbon Nanotubes. ACS Nano, 2010, 4, 7596-7602.	14.6	133
113	Donor levels in Si nanowires determined by hybrid-functional calculations. Physical Review B, 2009, 79, .	3.2	28
114	Theory of Defects in One-Dimensional Systems: Application to Al-Catalyzed Si Nanowires. Nano Letters, 2009, 9, 975-979.	9.1	62
115	Using Thermal Gradients for Actuation in the Nanoscale. IUTAM Symposium on Cellular, Molecular and Tissue Mechanics, 2009, , 141-150.	0.2	0
116	Transport in silicon nanowires: role of radial dopant profile. Journal of Computational Electronics, 2008, 7, 324-327.	2.5	15
117	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
118	Band bending and quasiâ€2DEG in the metallized Î²â€SiC(001) surface. Physica Status Solidi - Rapid Research Letters, 2008, 2, 218-220.	2.4	9
119	Subnanometer Motion of Cargoes Driven by Thermal Gradients Along Carbon Nanotubes. Science, 2008, 320, 775-778.	12.6	322
120	Modeling Transport in Ultrathin Si Nanowires: Charged versus Neutral Impurities. Nano Letters, 2008, 8, 2825-2828.	9.1	34
121	The BN-pair impurity in carbon nanotubes and the possibility for disorder-induced frustration of gap formation. Nanotechnology, 2008, 19, 445709.	2.6	6
122	Large electromechanical response in silicon nanowires predicted from first-principles electronic structure calculations. Physical Review B, 2008, 77, .	3.2	4
123	Mn-doped silicon nanowires: First-principles calculations. Physical Review B, 2008, 78, .	3.2	14
124	Fabrication of ordered arrays of quantum wires through hole patterning. Journal of Physics: Conference Series, 2008, 100, 052049.	0.4	1
125	Structural and electronic properties of zigzag carbon nanotubes filled with small fullerenes. Journal of Physics Condensed Matter, 2007, 19, 236222.	1.8	15
126	Ferrodistortive Instability at the (001) Surface of Half-Metallic Manganites. Physical Review Letters, 2007, 99, 226101.	7.8	40

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127	Ordered arrays of quantum wires through hole patterning: ab initio and empirical electronic structure calculations. Applied Physics Letters, 2007, 90, 083118.	3.3	8
128	Accurate single-particle determination of the band gap in silicon nanowires. Physical Review B, 2007, 76, .	3.2	39
129	Scaling Theory Put into Practice: First-Principles Modeling of Transport in Doped Silicon Nanowires. Physical Review Letters, 2007, 99, 076803.	7.8	112
130	Molecular orbital shift of perylenetetracarboxylic-dianhydride on gold. Chemical Physics Letters, 2007, 438, 249-253.	2.6	63
131	Spontaneous Formation of Triptycene Supramolecules on Surfaces. Journal of Physical Chemistry B, 2006, 110, 20089-20092.	2.6	10
132	Molecules on vicinal Au surfaces studied by scanning tunnelling microscopy. Journal of Physics Condensed Matter, 2006, 18, S51-S66.	1.8	17
133	Electronic transport through Si nanowires: Role of bulk and surface disorder. Physical Review B, 2006, 74, .	3.2	95
134	Prediction of giant electroactuation for papyruslike carbon nanoscroll structures: First-principles calculations. Physical Review B, 2006, 74, .	3.2	63
135	Size effects in surface-reconstructedâŸ¨100âŸ©andâŸ¨110âŸ©silicon nanowires. Physical Review B, 2006, 74, .	3.2	37
136	Electron Transport via Local Polarons at Interface Atoms. Physical Review Letters, 2006, 97, 206801.	7.8	50
137	On the properties of surface reconstructed silicon nanowires. Nanotechnology, 2005, 16, S250-S253.	2.6	32
138	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
139	First stages of the oxidation of the Si-rich 3Câ€“SiC(001) surface. Computational Materials Science, 2005, 33, 13-19.	3.0	9
140	Single-molecule manipulation and chemistry with the STM. Journal of Physics Condensed Matter, 2005, 17, S1049-S1074.	1.8	62
141	Metallic and Semimetallic SiliconâŸ¨100âŸ©Nanowires. Physical Review Letters, 2005, 94, 026805.	7.8	164
142	Electronic and structural properties of silicon carbide nanowires. Physical Review B, 2005, 71, .	3.2	63
143	Prediction of Ordered Phases of Encapsulated C60, C70, and C78Inside Carbon Nanotubes. Nano Letters, 2005, 5, 349-355.	9.1	85
144	Reversible scaling simulations of the melting transition in silicon. Physical Review B, 2004, 69, .	3.2	19

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145	First-Principles Study of O Adsorption at SiC Surface. Materials Science Forum, 2004, 457-460, 1293-1296.	0.3	3
146	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
147	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
148	First-principles studies of the diffusion of B impurities and vacancies in SiC. Physical Review B, 2004, 69, .	3.2	24
149	Charge corrections for supercell calculations of defects in semiconductors. Physica B: Condensed Matter, 2003, 340-342, 190-194.	2.7	60
150	Fullerene Coalescence in Nanopeapods:â€‰ A Path to Novel Tubular Carbon. Nano Letters, 2003, 3, 1037-1042.	9.1	185
151	First principles studies of neutral vacancies diffusion in SiC. Computational Materials Science, 2003, 27, 36-42.	3.0	18
152	Trocadero: a multiple-algorithm multiple-model atomistic simulation program. Computational Materials Science, 2003, 28, 85-106.	3.0	75
153	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
154	First-principles study of n-type dopants and their clustering in SiC. Applied Physics Letters, 2003, 82, 4298-4300.	3.3	24
155	Theoretical evidence for the kick-out mechanism for B diffusion in SiC. Applied Physics Letters, 2002, 81, 2989-2991.	3.3	26
156	Ab Initio Calculations of B Diffusion in SiC. Materials Science Forum, 2002, 389-393, 553-556.	0.3	1
157	An experimental test on the distribution of positronium lifetimes in polymers. Chemical Physics, 1998, 237, 493-499.	1.9	18