Keivan Esfarjani

List of Publications by Year
in descending order

153 papers	10,275 citations	50276 46 h-index	32842 100 g-index
155 all docs	155 docs citations	155 times ranked	8522 citing authors

#	Article	IF	Citations
1	Low-resistance contact in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoSe</mml:mi><mml:mn>2</mml:mn></mml:msub><m -based solid-state thermionic devices. Physical Review B, 2022, 105, .	3.2	2
2	Ab initio phonon transport across grain boundaries in graphene using machine learning based on small dataset. Physical Review Materials, 2022, 6, .	2.4	0
3	Calculation of thermomagnetic properties using first-principles density functional theory. Computational Materials Science, 2022, 210, 111412.	3.0	4
4	Thermomagnetic properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Bi</mml:mi><mml:mn>2</mml:mn></mml:m single crystal in the temperature range from 55ÂK to 380 K. Physical Review Materials, 2021, 5, .	2.4	8
5	Tunable lattice distortion in MgCoNiCuZnO5 entropy-stabilized oxide. Journal of Materials Research, 2021, 36, 1615-1623.	2.6	3
6	Nernst coefficient within relaxation time approximation. Physical Review B, 2021, 103, .	3.2	8
7	Effect of exchange-correlation functional type and spin-orbit coupling on thermoelectric properties of ZrTe2. Journal of Solid State Chemistry, 2021, 302, 122414.	2.9	6
8	Theory of Non-Equilibrium Heat Transport in Anharmonic Multiprobe Systems at High Temperatures. Entropy, 2021, 23, 1630.	2.2	1
9	Ultra-high lattice thermal conductivity and the effect of pressure in superhard hexagonal BC₂N. Journal of Materials Chemistry C, 2020, 8, 15705-15716.	5.5	6
10	Evidence for pseudoâ€“Jahn-Teller distortions in the charge density wave phase of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>1</mml:mn><mml:mi>T</mml:mi><mml:mtext> Physical Review B, 2020, 101, .	3.2	25
11	Delocalization of phonons and energy spectrum in disordered nonlinear systems. Physical Review B, 2020, 101, .	3.2	0
12	The thermal and mechanical properties of hafnium orthosilicate: Experiments and first-principles calculations. Materialia, 2020, 12, 100793.	2.7	23
13	Improved Thermoelectric Performance of Ecoâ€Friendly Î²â€FeSi 2 â€“SiGe Nanocomposite via Synergistic Hierarchical Structuring, Phase Percolation, and Selective Doping. Advanced Functional Materials, 2019, 29, 1903157.	14.9	27
14	Unexpectedly high cross-plane thermoelectric performance of layered carbon nitrides. Journal of Materials Chemistry A, 2019, 7, 2114-2121.	10.3	44
15	Novel MAB phases and insights into their exfoliation into 2D MBenes. Nanoscale, 2019, 11, 11305-11314.	5.6	120
16	Non-linear enhancement of thermoelectric performance of a TiSe₂ monolayer due to tensile strain, from first-principles calculations. Journal of Materials Chemistry C, 2019, 7, 7308-7317.	5.5	22
17	Thermoelectric properties of semimetals. Physical Review Materials, 2019, 3, .	2.4	47
18	Insights into exfoliation possibility of MAX phases to MXenes. Physical Chemistry Chemical Physics, 2018, 20, 8579-8592.	2.8	182

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19	Ab Initio Methods. , 2018, , 7-197.		2
20	Semi-metals as potential thermoelectric materials. Scientific Reports, 2018, 8, 9876.	3.3	71
21	Thermal management and non-reciprocal control of phonon flow via optomechanics. Nature Communications, 2018, 9, 1207.	12.8	48
22	High-Performance Solid-State Thermionic Energy Conversion Based on 2D van der Waals Heterostructures: A First-Principles Study. Scientific Reports, 2018, 8, 9303.	3.3	21
23	Phonon scattering effects from point and extended defects on thermal conductivity studied via ion irradiation of crystals with self-impurities. Physical Review Materials, 2018, 2, .	2.4	22
24	Tight-Binding Methods. , 2018, , 199-230.		0
25	Cross-Plane Seebeck Coefficient Measurement of Misfit Layered Compounds (SnSe)_n(TiSe₂)_n (n = 1,3,4,5). Nano Letters, 2017, 17, 1978-1986.	9.1	25
26	First-Principles Calculation of Charge Transfer at the Siliconâ€“Organic Interface. Journal of Physical Chemistry C, 2017, 121, 15529-15537.	3.1	10
27	Temperature-dependent thermal conductivity in silicon nanostructured materials studied by the Boltzmann transport equation. Physical Review B, 2016, 93, .	3.2	44
28	Molecular Dynamics Study of Cubic Boron Nitride Nanoparticles: Decomposition with Phase Segregation during Melting. ACS Nano, 2016, 10, 10563-10572.	14.6	15
29	First principles calculations of solid-state thermionic transport in layered van der Waals heterostructures. Nanoscale, 2016, 8, 14695-14704.	5.6	33
30	Gap tuning and effective electron correlation energy in amorphous silicon: A first principles density functional theory-based molecular dynamics study. Computational Materials Science, 2015, 102, 110-118.	3.0	3
31	Significant Reduction of Lattice Thermal Conductivity by the Electron-Phonon Interaction in Silicon with High Carrier Concentrations: A First-Principles Study. Physical Review Letters, 2015, 114, 115901.	7.8	229
32	Thermal Interface Conductance Between Aluminum and Silicon by Molecular Dynamics Simulations. Journal of Computational and Theoretical Nanoscience, 2015, 12, 168-174.	0.4	78
33	Hydrodynamic phonon transport in suspended graphene. Nature Communications, 2015, 6, 6290.	12.8	254
34	Abundance of Nanoclusters in a Molecular Beam: The Magic Numbers for Lennard-Jones Potential. Journal of Cluster Science, 2015, 26, 473-490.	3.3	6
35	Transition from near-field thermal radiation to phonon heat conduction at sub-nanometre gaps. Nature Communications, 2015, 6, 6755.	12.8	95
36	An ab initio study of multiple phonon scattering resonances in silicon germanium alloys. Journal of Applied Physics, 2015, 117, 174301.	2.5	9

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37	Ab initio optimization of phonon drag effect for lower-temperature thermoelectric energy conversion. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 14777-14782.	7.1	75
38	Lattice thermal conductivity of Bi, Sb, and Bi-Sb alloy from first principles. Physical Review B, 2014, 89, .	3.2	55
39	First-principles study of thermal transport inFeSb2. Physical Review B, 2014, 89, .	3.2	23
40	Green's function studies of phonon transport across Si/Ge superlattices. Physical Review B, 2014, 89, .	3.2	60
41	Resonant bonding leads to low lattice thermal conductivity. Nature Communications, 2014, 5, 3525.	12.8	484
42	First principles molecular dynamics studies of elastic constants, ideal tensile strength, chemistry of crack initiation, and surface and cohesive energies in amorphous silicon. Philosophical Magazine, 2014, 94, 2913-2936.	1.6	8
43	MODELING HEAT CONDUCTION FROM FIRST PRINCIPLES. Annual Review of Heat Transfer, 2014, 17, 9-47.	1.0	17
44	Gallium arsenide thermal conductivity and optical phonon relaxation times from first-principles calculations. Europhysics Letters, 2013, 101, 16001.	2.0	100
45	Enhancing the Thermoelectric Power Factor by Using Invisible Dopants. Advanced Materials, 2013, 25, 1577-1582.	21.0	61
46	Lifetime of sub-THz coherent acoustic phonons in a GaAs-AlAs superlattice. Applied Physics Letters, 2013, 102, .	3.3	41
47	High thermoelectric performance by resonant dopant indium in nanostructured SnTe. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 13261-13266.	7.1	632
48	Metallic Composites Phase-Change Materials for High-Temperature Thermal Energy Storage. , 2013, , .		1
49	Isotropic and energy-selective electron cloaks on graphene. Physical Review B, 2013, 88, .	3.2	30
50	Non-diffusive relaxation of a transient thermal grating analyzed with the Boltzmann transport equation. Journal of Applied Physics, 2013, 114, 104302.	2.5	58
51	Importance of local force fields on lattice thermal conductivity reduction in PbTe 1âˆ'x Se x alloys. Europhysics Letters, 2013, 102, 46002.	2.0	39
52	Microscopic mechanism of low thermal conductivity in lead telluride. Physical Review B, 2012, 85, .	3.2	115
53	Coherent Phonon Heat Conduction in Superlattices. Science, 2012, 338, 936-939.	12.6	489
54	Thermal interface conductance in Si/Ge superlattices by equilibrium molecular dynamics. Physical Review B, 2012, 85, .	3.2	128

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55	Interfacial Water Facilitates Energy Transfer by Inducing Extended Vibrations in Membrane Lipids. Journal of Physical Chemistry B, 2012, 116, 6455-6460.	2.6	15
56	Enhancing phonon transmission across a Si/Ge interface by atomic roughness: First-principles study with the Green's function method. Physical Review B, 2012, 86, .	3.2	232
57	Cloaking Core-Shell Nanoparticles from Conducting Electrons in Solids. Physical Review Letters, 2012, 109, 126806.	7.8	58
58	Study of the Thermoelectric Properties of Lead Selenide Doped with Boron, Gallium, Indium, or Thallium. Journal of the American Chemical Society, 2012, 134, 17731-17738.	13.7	105
59	Enhancement of thermoelectric figure-of-merit by resonant states of aluminium doping in lead selenide. Energy and Environmental Science, 2012, 5, 5246-5251.	30.8	372
60	Stronger phonon scattering by larger differences in atomic mass and size in p-type half-Heuslers Hf1â^'xTixCoSb0.8Sn0.2. Energy and Environmental Science, 2012, 5, 7543.	30.8	244
61	Phonon conduction in PbSe, PbTe, and PbTe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^'</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>Se<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>x</mml:mi></mml:msub></mml:math>from first-principles calculations. Physical Review B, 2012, 85, .	3.2	463
62	Perspectives on thermoelectrics: from fundamentals to device applications. Energy and Environmental Science, 2012, 5, 5147-5162.	30.8	1,080
63	Thermal Conductivity Spectroscopy Technique to Measure Phonon Mean Free Paths. Physical Review Letters, 2011, 107, 095901.	7.8	438
64	Low-Temperature Thermoelectric Power Factor Enhancement by Controlling Nanoparticle Size Distribution. Nano Letters, 2011, 11, 225-230.	9.1	56
65	Molecular dynamics simulation of thermal energy transport in polydimethylsiloxane. Journal of Applied Physics, 2011, 109, .	2.5	87
66	On the importance of optical phonons to thermal conductivity in nanostructures. Applied Physics Letters, 2011, 99, .	3.3	137
67	Many-electron states of nitrogen-vacancy centers in diamond and spin density calculations. Physical Review B, 2011, 84, .	3.2	27
68	Heat transport in silicon from first-principles calculations. Physical Review B, 2011, 84, .	3.2	618
69	Thermal Conductivity of Cage-Like Structures. , 2011, , .		0
70	High-pressure phases of hydrogen cyanide: formation of hydrogenated carbon nitride polymers and layers and their electronic properties. Journal of Physics Condensed Matter, 2011, 23, 405403.	1.8	11
71	Thermal conductivity of half-Heusler compounds from first-principles calculations. Physical Review B, 2011, 84, .	3.2	187
72	First-Principles-Based Interatomic Potential for SI and Its Thermal Conductivity. , 2011, , .		0

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73	Cluster scattering effects on phonon conduction in graphene. Physical Review B, 2010, 81, .	3.2	93
74	Effect of filler mass and binding on thermal conductivity of fully filled skutterudites. Physical Review B, 2010, 82, .	3.2	21
75	Strain-induced instability of spherical nanodiamond hydrocarbons: Effect of surface<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CH</mml:mtext></mml:mrow><mml:mi>n</mml:mi></mml:msub> charging. Physical Review B, 2009, 79, .	3.2	6
76	Effect of Nanoparticles on Electron and Thermoelectric Transport. Journal of Electronic Materials, 2009, 38, 954-959.	2.2	32
77	Effect of nanoparticle scattering on thermoelectric power factor. Applied Physics Letters, 2009, 94, 202105.	3.3	124
78	Negative differential resistance in molecular junctions: Application to graphene ribbon junctions. Physical Review B, 2008, 78, .	3.2	42
79	Spin and band-gap engineering in doped graphene nanoribbons. Physical Review B, 2008, 78, .	3.2	128
80	Method to extract anharmonic force constants from first principles calculations. Physical Review B, 2008, 77, .	3.2	295
81	GROUND-STATE ENERGY AND COMPRESSIBILITY OF A DISORDERED TWO-DIMENSIONAL ELECTRON GAS. International Journal of Modern Physics B, 2007, 21, 2134-2144.	2.0	2
82	Monte Carlo simulation of electron transport in degenerate and inhomogeneous semiconductors. Applied Physics Letters, 2007, 90, 092111.	3.3	23
83	Enhanced Cooling in Doped Semiconductors Due to Nonlinear Peltier Effect. Materials Research Society Symposia Proceedings, 2007, 1044, 1.	0.1	3
84	Nonlinear Peltier effect in semiconductors. Applied Physics Letters, 2007, 91, 122104.	3.3	44
85	Spin dynamics characterization in magnetic dots. Physica B: Condensed Matter, 2007, 399, 81-93.	2.7	6
86	GROUND-STATE ENERGY AND COMPRESSIBILITY OF A DISORDERED TWO-DIMENSIONAL ELECTRON GAS. , 2007, , .		0
87	Thermoelectric transport perpendicular to thin-film heterostructures calculated using the Monte Carlo technique. Physical Review B, 2006, 74, .	3.2	42
88	Molecular dynamics of single wall carbon nanotube growth on nickel surface. Computational Materials Science, 2006, 36, 117-120.	3.0	10
89	Generalized Hubbard model for many-electron states of the diamond vacancies: A non-CI approach. Physica Status Solidi (B): Basic Research, 2006, 243, 1269-1275.	1.5	1
90	Relationship between lattice relaxation and electron delocalization in diamond vacancies. Physica B: Condensed Matter, 2006, 376-377, 324-326.	2.7	2

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91	Thermoelectric properties of a nanocontact made of two-capped single-wall carbon nanotubes calculated within the tight-binding approximation. Physical Review B, 2006, 73, .	3.2	117
92	Coherent conductance in an alternating dot: exact results. Physica E: Low-Dimensional Systems and Nanostructures, 2005, 27, 227-234.	2.7	15
93	Spin filtering and spin diode devices in quantum wire systems. Physica E: Low-Dimensional Systems and Nanostructures, 2005, 27, 325-331.	2.7	51
94	Analytical results on coherent conductance in a general periodic quantum dot: Transfer matrix method. Physica E: Low-Dimensional Systems and Nanostructures, 2005, 28, 150-161.	2.7	23
95	Properties of charge and magnetic impurities in a spin-polarized electron gas: A semiclassical approach. Physica E: Low-Dimensional Systems and Nanostructures, 2005, 28, 313-322.	2.7	1
96	Analytical results on ballistic transport in a periodic molecular wire. Chemical Physics, 2005, 317, 43-48.	1.9	8
97	Localization-delocalization transition in a one one-dimensional system with long-range correlated off-diagonal disorder. Physical Review B, 2005, 72, .	3.2	55
98	Lattice relaxation in many-electron states of the diamond vacancy. Physical Review B, 2005, 71, .	3.2	10
99	Nonlinear Charging and Transport Times in Doped Nanotubes Junctions. Journal of the Physical Society of Japan, 2005, 74, 515-518.	1.6	3
100	Oscillator strength calculations in color centers of diamond and the role of spin. European Physical Journal B, 2004, 39, 441-446.	1.5	6
101	Some analytical results in phase coherent transport in quantum wire. Physica E: Low-Dimensional Systems and Nanostructures, 2004, 25, 119-130.	2.7	20
102	Details of a theoretical model for electronic structure of the diamond vacancies. Diamond and Related Materials, 2004, 13, 2125-2130.	3.9	9
103	Electronic properties of magnetically doped nanotubes. Bulletin of Materials Science, 2003, 26, 105-107.	1.7	4
104	Screening at doped nanotube junctions beyond linear response. Physical Review B, 2002, 65, .	3.2	9
105	Ab Initio Computer Simulations on Microclusters: Structures and Electronic Properties. Springer Series in Cluster Physics, 2002, , 9-88.	0.3	16
106	Electron-interaction effects on transport characteristics of nanotubes. Physica B: Condensed Matter, 2002, 323, 242-243.	2.7	1
107	Statics and dynamics of phase segregation in multicomponent fermion gas. European Physical Journal D, 2002, 21, 181-189.	1.3	1
108	The Nanostructure of C60 Photopolymers. Springer Series in Cluster Physics, 2002, , 135-169.	0.3	7

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109	Electronic, Transport and Mechanical Properties of Carbon Nanotubes. Springer Series in Cluster Physics, 2002, , 187-220.	0.3	3
110	Charge oscillation at doped nanotube junctions. AIP Conference Proceedings, 2001, , .	0.4	0
111	Spin valve effect in magnetically doped nanotube-based transistors. AIP Conference Proceedings, 2001, , .	0.4	0
112	Effect of Elastic Interaction on Self-Assembled Island Spatial Arrangement. Materials Transactions, 2001, 42, 2279-2282.	1.2	0
113	Why the all-electron full-potential approach is suitable for calculations on fullerenes and nanotubes?. Journal of Molecular Graphics and Modelling, 2001, 19, 270-273.	2.4	3
114	Transport properties of a nanotube-based transistor. European Physical Journal D, 2001, 16, 353-355.	1.3	3
115	Realization of an effective ultrahigh magnetic field on a nanoscale. Journal of Physics Condensed Matter, 2001, 13, L49-L55.	1.8	4
116	Effect of inter-island interaction on the growth of self-assembled quantum dots. Springer Proceedings in Physics, 2001, , 389-390.	0.2	0
117	In Situ FTIR, XPS, and STM Studies of the Nano-Structure of a Photopolymerized C₆₀ Film. Molecular Crystals and Liquid Crystals, 2000, 340, 689-694.	0.3	8
118	Computational Materials Science. Springer Series in Solid-state Sciences, 1999, , .	0.3	85
119	Nonlinear Coherent Transport Through Doped Nanotube Junctions. Physical Review Letters, 1999, 82, 5084-5087.	7.8	124
120	In-situ infrared spectroscopy of a photoirradiated potassium-doped C60 film. Chemical Physics Letters, 1999, 315, 19-24.	2.6	22
121	Fourier transform infrared and mass spectrometry studies of a photoirradiated KxC60 film. European Physical Journal D, 1999, 9, 363-367.	1.3	2
122	The three-fermion problem in two and three dimensions; a unified variational approach. Journal of Physics B: Atomic, Molecular and Optical Physics, 1999, 32, 749-756.	1.5	3
123	Ab Initio study of dopant insertion into carbon nanotubes. Journal of Chemical Physics, 1999, 111, 2164-2168.	3.0	44
124	Electronic and transport properties of N-P doped nanotubes. Applied Physics Letters, 1999, 74, 79-81.	3.3	100
125	Localized basis set optimization. Computational Materials Science, 1999, 15, 351-356.	3.0	3
126	Ab Initio Methods. Springer Series in Solid-state Sciences, 1999, , 7-138.	0.3	5

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127	Tight-Binding Methods. Springer Series in Solid-state Sciences, 1999, , 139-170.	0.3	0
128	Fourier transform infrared and mass spectrometry studies of a photoirradiated KxC60 film. , 1999, , 363-367.		0
129	Tight-binding parametrization of transition metal elements from LCAO ab initio Hamiltonians. Computational Materials Science, 1998, 9, 343-347.	3.0	5
130	Client-server model of integrated production facilities. International Journal of Production Research, 1998, 36, 3295-3321.	7.5	22
131	Self-consistent tight-binding formalism for charged systems. Journal of Physics Condensed Matter, 1998, 10, 8257-8267.	1.8	39
132	Vibrational modes and IR analysis of neutral photopolymerizedC60dimers. Physical Review B, 1998, 57, 223-229.	3.2	62
133	An All-electron First-principles Molecular Dynamics Method and a Possibility of its Application to Atomistically Distorted Systems. Advances in Materials Research, 1998, , 210-219.	0.2	5
134	Molecular dynamics simulation on aligning process of C[sub 60] on various substrates and the origin of specific surface electronic states. , 1997, , .		0
135	Simulated annealing of small silicon clusters by tight-binding. , 1997, , .		0
136	Stability and vibrational spectra of toroidal isomers of C_{240}. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1997, 41, 73-76.	1.0	3
137	Effect of orientation on the band structure of C58BN hetero-fullerenes in fcc solid phase. Solid State Communications, 1996, 97, 539-542.	1.9	12
138	Ab InitioMolecular Dynamics Simulations for Collision betweenC60â^'and Alkali-Metal Ions: A Possibility of Li@C60. Physical Review Letters, 1996, 76, 3590-3593.	7.8	85
139	ELECTRONIC PROPERTIES OF C58BN HETEROFULLERENES. Surface Review and Letters, 1996, 03, 747-752.	1.1	7
140	Phase Stability of the Sigma Phase in Fe-Cr Based Alloys. Materials Research Society Symposia Proceedings, 1995, 408, 369.	0.1	0
141	Site Occupation Reversal in theFeâ^'CrÏƒPhase. Physical Review Letters, 1995, 75, 3142-3145.	7.8	72
142	A bilayer of Wigner crystal in the harmonic approximation. Journal of Physics Condensed Matter, 1995, 7, 7217-7226.	1.8	18
143	Band structure and chemical bonding inC58BN heterofullerenes. Physical Review B, 1994, 50, 17830-17836.	3.2	53
144	Electronic Properties of C58Bn Fullerenes. Materials Research Society Symposia Proceedings, 1994, 349, 225.	0.1	0

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145	Search for the Ground State of C60B10. Materials Research Society Symposia Proceedings, 1994, 359, 229.	0.1	0
146	Dislocation waves in a two-dimensional Coulomb lattice. Physical Review B, 1992, 46, 4638-4643.	3.2	11
147	Shear modulus of the magnetophonon wave function. Solid State Communications, 1991, 79, 387-388.	1.9	7
148	Self-consistent phonon and magnetophonon and cubic anharmonic corrections of the 2D electron lattice. Journal of Physics Condensed Matter, 1991, 3, 5825-5836.	1.8	17
149	Finite-temperature two-dimensional Wigner transition. Physical Review B, 1991, 44, 11498-11501.	3.2	22
150	Finite-temperature transport of a pinned 2D electron lattice. Physical Review Letters, 1991, 66, 652-654.	7.8	33
151	A Mechanism for Quantum Melting in Two Dimensions. Europhysics Letters, 1991, 14, 361-365.	2.0	42
152	Solidification of the two-dimensional electron gas in high magnetic fields. Physical Review B, 1990, 42, 10758-10760.	3.2	42
153	Disorder, screening, and quantum Hall oscillations. Physical Review B, 1990, 41, 1042-1053.	3.2	29