

J A VergÃ©s

List of Publications by Year in descending order

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102
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103
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103
docs citations

103
times ranked

1643
citing authors

#	ARTICLE	IF	CITATIONS
1	First-principles approach to electrical transport in atomic-scale nanostructures. Physical Review B, 2002, 66, .	1.1	186
2	First-Principles Phase-Coherent Transport in Metallic Nanotubes with Realistic Contacts. Physical Review Letters, 2003, 90, 106801.	2.9	159
3	Strong covalent bonding between two graphene layers. Physical Review B, 2008, 77, .	1.1	147
4	Fullerene-based molecular nanobridges: a first-principles study. Physical Review B, 2001, 64, .	1.1	138
5	Holes and magnetic textures in the two-dimensional Hubbard model. Physical Review B, 1991, 43, 6099-6108.	1.1	129
6	Absolute Hydrostatic Deformation Potentials of Tetrahedral Semiconductors. Physica Status Solidi (B): Basic Research, 1982, 113, 519-534.	0.7	89
7	Hydrogen on graphene under stress: Molecular dissociation and gap opening. Physical Review B, 2010, 81, .	1.1	77
8	Implementing the Keldysh formalism into ab initio methods for the calculation of quantum transport: Application to metallic nanocontacts. Physical Review B, 2003, 67, .	1.1	76
9	Lattice-Spin Mechanism in Colossal Magnetoresistive Manganites. Physical Review Letters, 2002, 88, 136401.	2.9	64
10	Ab initio self-consistent calculation of silicon electronic structure by means of Wannier functions. Physical Review B, 1979, 19, 2283-2290.	1.1	59
11	Electronic structure, defect states, and optical absorption of amorphous $\text{Si}_{1-x}\text{N}_x$ [$0 \leq x/(1-x) \leq 2$]. Physical Review B, 1987, 35, 9683-9692.	1.1	58
12	First-principles calculation of the effect of stress on the chemical activity of graphene. Applied Physics Letters, 2008, 93, .	1.5	50
13	Electronic transport and vibrational modes in a small molecular bridge: H_2 in Pt nanocontacts. Physical Review B, 2004, 69, .	1.1	48
14	Transport regimes in surface disordered graphene sheets. Physical Review B, 2007, 75, .	1.1	46
15	Model of Quantum Chaotic Billiards: Spectral Statistics and Wave Functions in Two Dimensions. Physical Review Letters, 1996, 77, 1970-1973.	2.9	43
16	Holes and Magnetic Textures in the Two-Dimensional Hubbard Model. Europhysics Letters, 1991, 14, 157-163.	0.7	39
17	Ab initio electronic and geometrical structures of tripotassium-intercalated phenanthrene. Physical Review B, 2011, 84, .	1.1	34
18	Electronic transport through C_{60} molecules. Nanotechnology, 2001, 12, 160-163.	1.3	31

#	ARTICLE	IF	CITATIONS
19	Conductance as a function of temperature in the double-exchange model. Physical Review B, 1999, 59, 4170-4175.	1.1	29
20	Unrestricted Hartree-Fock study of the two-band Hamiltonian in dopedCuO ₂ planes. Physical Review B, 1992, 46, 3562-3572.	1.1	26
21	Self-consistent localised description of the electronic structure of semiconductors. Journal of Physics C: Solid State Physics, 1979, 12, 499-511.	1.5	25
22	Bethe Lattices Incorporating Short-Range Disorder: Application to Hydrogenated Amorphous Silicon. Physical Review Letters, 1984, 53, 2270-2273.	2.9	25
23	Random-Bethe-lattice model applied to the electronic structure of amorphous and liquid silicon. Physical Review B, 1990, 42, 7193-7203.	1.1	25
24	Fit of Pariser-Parr-Pople and Hubbard model Hamiltonians to charge and spin states of polycyclic aromatic hydrocarbons. Physical Review B, 2010, 81, .	1.1	25
25	Scaling of the Hamiltonian and momentum in semiconductors. Physical Review B, 1984, 29, 6840-6845.	1.1	24
26	Localization length in a random magnetic field. Physical Review B, 1998, 57, 870-878.	1.1	23
27	Self-consistent calculation of the structural properties of silicon. Physical Review B, 1979, 20, 4251-4255.	1.1	22
28	Self-energies of phonons in heavily dopedn- andp-type silicon. Physical Review B, 1982, 26, 5658-5667.	1.1	22
29	Self-similar magnetoconductance fluctuations in quantum dots. Physical Review B, 2000, 61, 13014-13020.	1.1	22
30	Hubbard Hamiltonian for the hydrogen molecule. Physical Review B, 2007, 75, .	1.1	21
31	Generalized Wannier functions at interfaces: Stacking faults in silicon. Physical Review B, 1981, 24, 1006-1013.	1.1	20
32	Configuration-interaction approach to hole pairing in the two-dimensional Hubbard model. Physical Review B, 1999, 59, 14005-14016.	1.1	19
33	Trapping of electrons near chemisorbed hydrogen on graphene. Physical Review B, 2010, 81, .	1.1	18
34	Transport through an interacting system connected to leads. Journal of Physics Condensed Matter, 2003, 15, 8805-8826.	0.7	17
35	Self-consistent calculation of the internal strain parameter of silicon. Physical Review B, 1982, 26, 5960-5962.	1.1	16
36	Possibility of finding reliable solid-state tight-binding parameters for the Si-N bond through quantum-chemistry calculations. Physical Review B, 1989, 39, 1844-1855.	1.1	16

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37	Electron states at steps in transition metal surfaces: A cluster-Bethe lattice approximation. Journal of Physics F: Metal Physics, 1978, 8, 873-881.	1.6	15
38	Disordered alloys with a Bethe lattice structure: a study of a new mean-field approximation. Journal of Physics C: Solid State Physics, 1987, 20, 5501-5515.	1.5	14
39	Excitations and response functions of the doped two-dimensional Hubbard model: A random-phase-approximation analysis. Physical Review B, 1992, 45, 4752-4758.	1.1	14
40	Mean free path and energy fluctuations in quantum chaotic billiards. Physical Review B, 1997, 56, 2120-2126.	1.1	14
41	Magnetic molecules created by hydrogenation of polycyclic aromatic hydrocarbons. Physical Review B, 2009, 79, .	1.1	14
42	Lattice defects in III-V semiconductors. Physical Review B, 1981, 24, 6020-6028.	1.1	13
43	Perturbation theory of the Hubbard Hamiltonian on a $4\tilde{A}-4$ cluster of the square lattice. Physical Review B, 1991, 44, 10093-10100.	1.1	13
44	Nonconventional behavior of the one-band Hubbard Hamiltonian in two dimensions. Physical Review B, 1992, 46, 3163-3166.	1.1	13
45	Second-order self-energy of the Hubbard Hamiltonian: Absence of quasiparticle excitations near half-filling. Physical Review B, 1993, 48, 13654-13660.	1.1	13
46	Topology-induced many body effects in hydrogenated Pt nanocontacts. Physical Review B, 2005, 71, .	1.1	13
47	Quantum chaos induced by scaled disorder. Physical Review E, 1999, 59, R3803-R3806.	0.8	11
48	Electronic density of states on a randomly dilute Cayley tree. Journal of Physics C: Solid State Physics, 1986, 19, 6751-6760.	1.5	10
49	Minimal tight-binding Hamiltonian for semiconductors. Physical Review B, 1988, 37, 4333-4336.	1.1	10
50	Chaotic behavior induced by point contacts in quantum dots. Physical Review B, 1998, 58, R10143-R10146.	1.1	10
51	Can model Hamiltonians describe the electron-electron interaction in π -conjugated systems?: PAH and graphene. Journal of Physics Condensed Matter, 2015, 27, 463001.	0.7	10
52	A simple tight-binding model for deep impurity levels: application to the Jahn-Teller-distorted nitrogen donor in silicon. Journal of Physics C: Solid State Physics, 1981, 14, 365-373.	1.5	9
53	Wave-function renormalization constant for the one-band Hubbard Hamiltonian in two dimensions. Physical Review B, 1993, 48, 426-436.	1.1	9
54	Surface Green functions approach to planar defects and surfaces in copper: twin faults and (100) and (111) surfaces. Journal of Physics F: Metal Physics, 1980, 10, 207-223.	1.6	8

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55	Effect of under- and overcoordination on the electronic structure of amorphous silicon. Physical Review B, 1989, 39, 3445-3448.	1.1	8
56	Holes and Magnetic Textures in the One-and Two-Band Hamiltonians for CuO ₂ Planes of High-T _c Superconductors. Physica Scripta, 1991, T39, 140-147.	1.2	8
57	Spin and Charge Excitations Induced by Holes in the Hubbard Model. Europhysics Letters, 1992, 17, 455-462.	0.7	8
58	Energy fluctuations, Thouless energy, and conductance in the Anderson model in the ballistic and diffusive regimes. Physical Review B, 1997, 56, 15853-15859.	1.1	8
59	Conductance scaling at the band center of wide wires with pure nondiagonal disorder. Physical Review B, 2001, 65, .	1.1	8
60	Spin alignment of extra electrons in K-phenanthrene clusters taken from the crystalline tripotassium-intercalated phenanthrene structure. Physical Review B, 2012, 85, .	1.1	8
61	Electronic structure of amorphous silicon carbide compounds. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1990, 61, 237-250.	0.6	7
62	Hole pairs in the two-dimensional Hubbard model. Europhysics Letters, 1998, 44, 229-234.	0.7	7
63	Transport regimes and critical energies in the two-dimensional Anderson model. Journal of Physics Condensed Matter, 1998, 10, 295-303.	0.7	7
64	Effects of Fermi energy, dot size, and leads width on weak localization in chaotic quantum dots. Physical Review B, 2001, 63, .	1.1	7
65	PPP Hamiltonian for polar polycyclic aromatic hydrocarbons. European Physical Journal B, 2011, 81, 253-262.	0.6	7
66	Conductance through the armchair graphene nanoribbons 9-AGNR: Strong dependence on contact to leads. Physical Review B, 2018, 98, .	1.1	7
67	Electronic structure of vacancies in Si(111) unreconstructed surfaces. Physical Review B, 1981, 23, 6676-6690.	1.1	6
68	Multiple-polaron description of the wave function of a single hole in Hubbard clusters of the square lattice. Physical Review B, 1993, 48, 9581-9585.	1.1	6
69	Effects of methods and basis set on ab initio calculations of electronic transport through hydrogenated Pt nanocontacts. International Journal of Quantum Chemistry, 2008, 108, 1637-1644.	1.0	6
70	Magnetism in hydrogenated and dehydrogenated benzene. Physica Status Solidi C: Current Topics in Solid State Physics, 2009, 6, 2139-2144.	0.8	6
71	Exponential decay of spin-spin correlation between distant defect states produced by contour hydrogenation of polycyclic aromatic hydrocarbon molecules. Physical Review B, 2013, 87, .	1.1	6
72	Analysis of the New Unrestricted Hartree-Fock Vortex Solution of the Hubbard Hamiltonian in Two-Dimensional Systems A Small Cluster Study. Physica Status Solidi (B): Basic Research, 1992, 173, 715-724.	0.7	5

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73	Quasiperiodic states in linear surface wave experiments. Philosophical Magazine, 2006, 86, 1065-1073.	0.7	5
74	Comment on "Critique of the tight-binding method: Ideal vacancy and surface states". Physical Review B, 1982, 26, 1059-1060.	1.1	4
75	Electronic structure of amorphousSi0.8Al0.2. Physical Review B, 1985, 32, 3662-3668.	1.1	4
76	Partially filled stripes in the two-dimensional Hubbard model: Statics and dynamics. Physical Review B, 2001, 64, .	1.1	4
77	A constructive definition of doubly occupied Wannier functions for metals; application to BCC Na. Journal of Physics F: Metal Physics, 1980, 10, 1167-1175.	1.6	3
78	Short- and long-range-order features in the electronic structure of bulk and surface vacancies in diamond-structure semiconductors. Physical Review B, 1981, 24, 3474-3480.	1.1	3
79	Dimensional effects in photoelectron spectra of Ag deposits on GaAs(110) surfaces. Physical Review B, 1996, 53, 6967-6970.	1.1	3
80	Wave-function and level statistics of random two-dimensional gauge fields. Physical Review B, 1996, 54, 14822-14832.	1.1	3
81	Correlation decay in quantum chaotic billiards with bulk or surface disorder. Physical Review E, 1999, 60, 391-397.	0.8	3
82	Classical trajectories in quantum transport at the band center of bipartite lattices with or without vacancies. Physical Review B, 2004, 69, .	1.1	3
83	Quasicrystalline and Rational Approximant Wave Patterns in Hydrodynamic and Quantum Nested Wells. Physical Review Letters, 2006, 97, 124501.	2.9	3
84	Generalized Wannier functions as a way to study the electron-phonon interaction in silicon. Physical Review B, 1984, 30, 2104-2111.	1.1	2
85	Global quantum fluctuations in metallic particles. Physical Review B, 1997, 56, R7045-R7048.	1.1	2
86	Electrical conductivity of a tight-binding hard-sphere model for hot fluid metals. Physical Review B, 2005, 71, .	1.1	2
87	Phase transitions due to the formation of polarons in colossal magnetoresistive manganites: Monte Carlo simulations. Physical Review B, 2006, 74, .	1.1	2
88	Electron correlation effects at vacancies in Si(111) unreconstructed surfaces. Physical Review B, 1984, 30, 1038-1041.	1.1	1
89	Surface Green function approach to the calculation of tunnelling currents in normal metal-superconductor junctions. Journal of Physics Condensed Matter, 1990, 2, 4143-4152.	0.7	1
90	Chaotic dynamics in an elastic medium with surface disorder. Physical Review E, 1997, 56, 4125-4129.	0.8	1

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91	Conductance fluctuations in metallic nanocontacts. Physical Review B, 2004, 70, .	1.1	1
92	Role of potassium orbitals in the metallic behavior of $K_3\text{picene}$. Physical Review B, 2014, 90, .	1.1	1
93	Short-Range Effects in Germanium-Silicon. Physica Status Solidi (B): Basic Research, 1980, 99, 501-505.	0.7	0
94	Electronic structure of line defects by means of the scattering theoretical method. Application to lines of vacancies in the simple cubic lattice. Physical Review B, 1983, 28, 4419-4425.	1.1	0
95	Dispersionless states in random Cayley trees with multiple connectivity. Physical Review B, 1987, 35, 9103-9107.	1.1	0
96	Unrestricted Hartree-Fock upper bounds for the total energy of the Hubbard model on a Bethe lattice of infinite connectivity. Physical Review B, 1994, 50, 13817-13820.	1.1	0
97	Medium/high-field magnetoconductance in chaotic quantum dots. Journal of Physics Condensed Matter, 2001, 13, 2935-2945.	0.7	0
98	A stripe with a local gate potential: An efficient magnetometer?. Physica Status Solidi (A) Applications and Materials Science, 2011, 208, 720-724.	0.8	0
99	Hartree Fock and RPA Studies of the Hubbard Model. NATO ASI Series Series B: Physics, 1995, , 295-302.	0.2	0
100	From One to Two Dimensions in the Weak Coupling Limit. NATO ASI Series Series B: Physics, 1995, , 303-306.	0.2	0
101	The Wavefunction Renormalization Constant for the One- and Two-Band Hubbard Hamiltonians in Two Dimensions. NATO ASI Series Series B: Physics, 1995, , 349-356.	0.2	0
102	Magnetoconductance in Chaotic Quantum Billiards. , 1999, , 69-78.		0