Daniel Kosov

List of Publications by Year
in descending order

93 papers	2,461 citations	257450 24 h-index	223800 46 g-index
94 all docs	94 docs citations	94 times ranked	1857 citing authors

#	Article	IF	Citations
1	Peptide conformational heterogeneity revealed from nonlinear vibrational spectroscopy and molecular-dynamics simulations. Journal of Chemical Physics, 2002, 117, 6833-6840.	3.0	219
2	Conformational Dynamics of Trialanine in Water. 2. Comparison of AMBER, CHARMM, GROMOS, and OPLS Force Fields to NMR and Infrared Experiments. Journal of Physical Chemistry B, 2003, 107, 5064-5073.	2.6	199
3	Convergence of the Electrostatic Interaction Based on Topological Atoms. Journal of Physical Chemistry A, 2001, 105, 8254-8261.	2.5	137
4	Ab initio-based exciton model of amide I vibrations in peptides: Definition, conformational dependence, and transferability. Journal of Chemical Physics, 2005, 122, 224904.	3.0	127
5	Atomic Partitioning of Molecular Electrostatic Potentials. Journal of Physical Chemistry A, 2000, 104, 7339-7345.	2.5	126
6	Atomâ€“atom partitioning of intramolecular and intermolecular Coulomb energy. Journal of Chemical Physics, 2001, 114, 6539-6547.	3.0	126
7	Convergence of the multipole expansion for electrostatic potentials of finite topological atoms. Journal of Chemical Physics, 2000, 113, 3969-3974.	3.0	79
8	Dithiocarbamate Anchoring in Molecular Wire Junctions:Â A First Principles Study. Journal of Physical Chemistry B, 2006, 110, 9893-9898.	2.6	78
9	Super-fermion representation of quantum kinetic equations for the electron transport problem. Journal of Chemical Physics, 2011, 134, 044121.	3.0	78
10	Nature of well-defined conductance of amine-anchored molecular junctions: Density functional calculations. Physical Review B, 2007, 76, .	3.2	74
11	Kohnâ€“Sham equations for nanowires with direct current. Journal of Chemical Physics, 2003, 119, 1-5.	3.0	53
12	Orbital Interaction Mechanisms of Conductance Enhancement and Rectification by Dithiocarboxylate Anchoring Group. Journal of Physical Chemistry B, 2006, 110, 19116-19120.	2.6	50
13	Consequences of covariant kaon dynamics in heavy ion collisions. Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics, 1998, 434, 245-250.	4.1	40
14	In-medium dependence and Coulomb effects of the pion production in heavy ion collisions. Nuclear Physics A, 1998, 628, 669-685.	1.5	37
15	Nonequilibrium perturbation theory in Liouvilleâ€“Fock space for inelastic electron transport. Journal of Physics Condensed Matter, 2012, 24, 225304.	1.8	35
16	Kramers problem for nonequilibrium current-induced chemical reactions. Journal of Chemical Physics, 2011, 135, 074701.	3.0	34
17	Out-of-equilibrium catalysis of chemical reactions by electronic tunnel currents. Journal of Chemical Physics, 2013, 138, 134103.	3.0	34
18	Origin of subthresholdK+production in heavy ion collisions. Physical Review C, 1997, 56, R606-R609.	2.9	33

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19	Constraints on the relativistic mean field of Î”-isobar in nuclear matter. Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics, 1998, 421, 37-40.	4.1	32
20	Plane wave/pseudopotential implementation of excited state gradients in density functional linear response theory: A new routevia implicit differentiation. Journal of Chemical Physics, 2005, 122, 144101.	3.0	32
21	SchrÃ¶dinger equation for current carrying states. Journal of Chemical Physics, 2002, 116, 6368-6375.	3.0	31
22	Spontaneous Sâ€“Si bonding of alkanethiols to Si(111)â€“H: towards Siâ€“moleculeâ€“Si circuits. Chemical Science, 2020, 11, 5246-5256.	7.4	30
23	Waiting time distribution for electron transport in a molecular junction with electron-vibration interaction. Journal of Chemical Physics, 2017, 146, 074102.	3.0	26
24	Scalar and vector decomposition of the nucleon self-energy in the relativistic Brueckner approach. Physical Review C, 1998, 58, 2022-2032.	2.9	25
25	Role of the Coulomb interaction in the flow and the azimuthal distribution of kaons from heavy ion reactions. Nuclear Physics A, 1998, 628, 151-160.	1.5	24
26	Stability analysis of multiple nonequilibrium fixed points in self-consistent electron transport calculations. Journal of Chemical Physics, 2011, 135, 174111.	3.0	24
27	Lagrange multiplier based transport theory for quantum wires. Journal of Chemical Physics, 2004, 120, 7165-7168.	3.0	23
28	Density functional calculations of 15N chemical shifts in solvated dipeptides. Journal of Biomolecular NMR, 2008, 41, 77-88.	2.8	22
29	Unified approach to the derivation of work theorems for equilibrium and steady-state, classical and quantum Hamiltonian systems. Physical Review E, 2008, 78, 011116.	2.1	22
30	Nonequilibrium Fock space for the electron transport problem. Journal of Chemical Physics, 2009, 131, 171102.	3.0	22
31	Nonequilibrium configuration interaction method for transport in correlated quantum systems. Journal of Physics A: Mathematical and Theoretical, 2014, 47, 095002.	2.1	21
32	Superoperator coupled cluster method for nonequilibrium density matrix. Journal of Physics A: Mathematical and Theoretical, 2015, 48, 015004.	2.1	21
33	Non-renewal statistics for electron transport in a molecular junction with electron-vibration interaction. Journal of Chemical Physics, 2017, 147, 104109.	3.0	21
34	Distribution of tunnelling times for quantum electron transport. Journal of Chemical Physics, 2016, 144, 124105.	3.0	20
35	Counting quantum jumps: A summary and comparison of fixed-time and fluctuating-time statistics in electron transport. Journal of Chemical Physics, 2019, 151, 034107.	3.0	20
36	Carâ€“Parrinello molecular dynamics on excited state surfaces. Journal of Chemical Physics, 1999, 110, 6645-6656.	3.0	16

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37	Molecular reorientation in hydrogen-bonding liquids: Through algebraic â^¼tâ^'3â^•2 relaxation toward exponential decay. Journal of Chemical Physics, 2006, 124, 144514.	3.0	16
38	Density functional calculations of chemical shielding of backbone 15N in helical residues of protein G. Journal of Biomolecular NMR, 2009, 45, 245-253.	2.8	16
39	Second-order post-Hartreeâ€“Fock perturbation theory for the electron current. Journal of Chemical Physics, 2011, 134, 154107.	3.0	16
40	Current-induced atomic motion, structural instabilities, and negative temperatures on molecule-electrode interfaces in electronic junctions. Physical Review B, 2020, 101, .	3.2	16
41	THE TFD TREATMENT OF THE QUASIPARTICLE-PHONON INTERACTION AT FINITE TEMPERATURE. Modern Physics Letters A, 1994, 09, 1735-1743.	1.2	15
42	Density functional calculations of backbone 15N shielding tensors in beta-sheet and turn residues of protein G. Journal of Biomolecular NMR, 2011, 50, 19-33.	2.8	14
43	Distribution of residence times as a marker to distinguish different pathways for quantum transport. Physical Review E, 2016, 94, 042134.	2.1	14
44	Anisotropy of SubthresholdK+Emission in Heavy Ion Reactions. Physical Review Letters, 1997, 79, 4096-4099.	7.8	13
45	Role of isospin dependent mean field in pion production in heavy ion reactions. Physical Review C, 1998, 57, 922-926.	2.9	13
46	Adsorption of lactic acid on chiral Pt surfacesâ€”A density functional theory study. Journal of Chemical Physics, 2013, 138, 084705.	3.0	13
47	Distribution of waiting times between electron cotunneling events. Physical Review B, 2018, 98, .	3.2	13
48	Nonrenewal statistics in quantum transport from the perspective of first-passage and waiting time distributions. Physical Review B, 2019, 99, .	3.2	13
49	What can be learned about molecular reorientation from single molecule polarization microscopy?. Journal of Chemical Physics, 2006, 125, 054708.	3.0	12
50	Doorwayâ€“window description of sequential three-pulse photon echo signals. Chemical Physics, 2008, 347, 177-184.	1.9	12
51	Solvent-induced current-voltage hysteresis and negative differential resistance in molecular junctions. Physical Review B, 2012, 85, .	3.2	12
52	Nonequilibrium Greenâ€™s function theory for nonadiabatic effects in quantum electron transport. Journal of Chemical Physics, 2017, 147, 224109.	3.0	12
53	Timescale separation solution of the Kadanoff-Baym equations for quantum transport in time-dependent fields. Physical Review B, 2019, 100, .	3.2	12
54	Waiting time between charging and discharging processes in molecular junctions. Journal of Chemical Physics, 2018, 149, 164105.	3.0	11

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55	Cooling molecular electronic junctions by AC current. Journal of Chemical Physics, 2020, 153, 121102.	3.0	11
56	First-passage time theory of activated rate chemical processes in electronic molecular junctions. Journal of Chemical Physics, 2021, 154, 114108.	3.0	11
57	Many-electron systems with constrained current. Physics Letters, Section A: General, Atomic and Solid State Physics, 2001, 291, 46-50.	2.1	10
58	Angular momentum dependent friction slows down rotational relaxation under nonequilibrium conditions. Journal of Chemical Physics, 2006, 125, 224502.	3.0	10
59	Asymptotic nonequilibrium steady-state operators. Physical Review E, 2009, 80, 022101.	2.1	10
60	Telegraph noise in Markovian master equation for electron transport through molecular junctions. Journal of Chemical Physics, 2018, 148, 184108.	3.0	10
61	RENORMALIZED RPA AT FINITE TEMPERATURE. Modern Physics Letters A, 1996, 11, 853-859.	1.2	9
62	First-principles calculations of conductance within a plane wave basis set via non-orthogonal Wannier-type atomic orbitals. Journal of Physics Condensed Matter, 2006, 18, 1347-1358.	1.8	9
63	Velocity dependence of friction and Kramers relaxation rates. Journal of Chemical Physics, 2007, 126, 244501.	3.0	9
64	Calculations of canonical averages from the grand canonical ensemble. Physical Review E, 2008, 77, 021120.	2.1	9
65	Non-adiabatic effects of nuclear motion in quantum transport of electrons: A self-consistent Keldyshâ€“Langevin study. Journal of Chemical Physics, 2020, 153, 154101.	3.0	9
66	Electronic statistics on demand: Bunching, antibunching, positive, and negative correlations in a molecular spin valve. Physical Review B, 2021, 103, .	3.2	9
67	A Markovian kinetic equation approach to electron transport through a quantum dot coupled to superconducting leads. Journal of Physics Condensed Matter, 2013, 25, 075702.	1.8	8
68	Decomposition of Ferrocene on Pt(111) and Its Effect on Molecular Electronic Junctions. Journal of Physical Chemistry C, 2019, 123, 15569-15574.	3.1	8
69	Microscopic origin of the jump diffusion model. Journal of Chemical Physics, 2009, 130, 134502.	3.0	7
70	Non-adiabatic corrections to electric current in molecular junctions due to nuclear motion at the molecule-electrode interfaces. Journal of Chemical Physics, 2018, 149, 044121.	3.0	7
71	Non-equilibrium Greenâ€™s function theory for non-adiabatic effects in quantum transport: Inclusion of electron-electron interactions. Journal of Chemical Physics, 2019, 150, 074101.	3.0	7
72	Fluctuating-time and full counting statistics for quantum transport in a system with internal telegraphic noise. Physical Review B, 2019, 100, .	3.2	7

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73	Silicon â˜’ single molecule â˜’ silicon circuits. Chemical Science, 2021, 12, 15870-15881.	7.4	7
74	Lindblad master equation approach to superconductivity in open quantum systems. Journal of Physics A: Mathematical and Theoretical, 2011, 44, 462001.	2.1	6
75	Conformation-dependent conductance through a molecular break junction. Journal of Molecular Modeling, 2013, 19, 4173-4180.	1.8	6
76	Full counting statistics for electron transport in periodically driven quantum dots. Physical Review B, 2020, 102, .	3.2	6
77	Approximate number projection at finite temperature. Zeitschrift FÃ¼r Physik A, 1996, 355, 17-21.	0.9	5
78	Enantioselectivity of (321) chiral noble metal surfaces: A density functional theory study of lactate adsorption. Journal of Chemical Physics, 2013, 139, 224709.	3.0	5
79	Linear response theory for symmetry improved two particle irreducible effective actions. Physical Review D, 2016, 93, .	4.7	5
80	Manifestation of nonequilibrium initial conditions in molecular rotation: The generalized J-diffusion model. Journal of Chemical Physics, 2007, 127, 144511.	3.0	4
81	A model for dynamical solvent control of molecular junction electronic properties. Journal of Chemical Physics, 2021, 154, 044107.	3.0	4
82	Self-similarity of single-channel transmission for electron transport in nanowires. Journal of Chemical Physics, 2006, 124, 104703.	3.0	3
83	Out-of-equilibrium one-dimensional disordered dipole chain. Physical Review E, 2013, 88, 012118.	2.1	3
84	Chiral selectivity of amino acid adsorption on chiral surfacesâ€"The case of alanine on Pt. Journal of Chemical Physics, 2015, 142, 054708.	3.0	3
85	Restoring the Pauli principle in the random phase approximation ground state. Chemical Physics Letters, 2017, 690, 20-24.	2.6	3
86	Self-consistent random-phase approximation for hot finite Fermi systems. Theoretical and Mathematical Physics(Russian Federation), 1997, 111, 613-620.	0.9	2
87	Adsorption and ring-opening of lactide on the chiral metal surface Pt(321)S studied by density functional theory. Journal of Chemical Physics, 2015, 142, 044703.	3.0	2
88	Coherent time-dependent oscillations and temporal correlations in triangular triple quantum dots. Physical Review B, 2021, 104, .	3.2	2
89	Expectation values of single-particle operators in the random phase approximation ground state. Journal of Chemical Physics, 2017, 146, 054103.	3.0	1
90	Self-consistent Hartree-Fock approximation for non-equilibrium electron transport through nanostructures. AIP Conference Proceedings, 2008, , .	0.4	0

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91	Directed motion and useful work from an isotropic nonequilibrium distribution. Physical Review E, 2008, 77, 011115.	2.1	0
92	Calculation of semiclassical free energy differences along nonequilibrium classical trajectories. Journal of Chemical Physics, 2009, 131, 164510.	3.0	0
93	Coupled elastic membranes model for quantum heat transport in semiconductor nanowires. European Physical Journal B, 2019, 92, 1.	1.5	0