Gianluca Stefanucci

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Time-dependent quantum transport: A practical scheme using density functional theory. Physical Review B, 2005, 72, .	3.2	291
2	Time-dependent partition-free approach in resonant tunneling systems. Physical Review B, 2004, 69, .	3.2	269
3	Kadanoff-Baym approach to quantum transport through interacting nanoscale systems: From the transient to the steady-state regime. Physical Review B, 2009, 80, .	3.2	186
4	A many-body approach to quantum transport dynamics: Initial correlations and memory effects. Europhysics Letters, 2008, 84, 67001.	2.0	134
5	Time-dependent quantum transport: An exact formulation based on TDDFT. Europhysics Letters, 2004, 67, 14-20.	2.0	121
6	Time-dependent approach to electron pumping in open quantum systems. Physical Review B, 2008, 77, .	3.2	115
7	Dynamical Coulomb Blockade and the Derivative Discontinuity of Time-Dependent Density Functional Theory. Physical Review Letters, 2010, 104, 236801.	7.8	115
8	Charge dynamics in molecular junctions: Nonequilibrium Green's function approach made fast. Physical Review B, 2014, 89, .	3.2	84
9	Towards a Description of the Kondo Effect Using Time-Dependent Density-Functional Theory. Physical Review Letters, 2011, 107, 216401.	7.8	83
10	Conserving approximations in time-dependent density functional theory. Physical Review B, 2005, 72, .	3.2	81
11	Bound states inab initioapproaches to quantum transport: A time-dependent formulation. Physical Review B, 2007, 75, .	3.2	77
12	Comparative study of many-body perturbation theory and time-dependent density functional theory in the out-of-equilibrium Anderson model. Physical Review B, 2011, 84, .	3.2	61
13	Time-dependent quantum transport with superconducting leads: A discrete-basis Kohn-Sham formulation and propagation scheme. Physical Review B, 2010, 81, .	3.2	58
14	Classical Nuclear Motion in Quantum Transport. Physical Review Letters, 2006, 97, 046603.	7.8	57
15	First-principles nonequilibrium Green's-function approach to transient photoabsorption: Application to atoms. Physical Review A, 2015, 92, .	2.5	57
16	First-principles approach to excitons in time-resolved and angle-resolved photoemission spectra. Physical Review B, 2016, 94, .	3.2	56
17	Time-dependent transport in graphene nanoribbons. Physical Review B, 2010, 82, .	3.2	53
18	Time-dependent Landauer-Büttiker formula: Application to transient dynamics in graphene nanoribbons. Physical Review B, 2014, 89, .	3.2	51

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19	Steady-State Density Functional Theory for Finite Bias Conductances. Nano Letters, 2015, 15, 8020-8025.	9.1	45
20	Dynamical Correction to Linear Kohn-Sham Conductances from Static Density Functional Theory. Physical Review Letters, 2013, 111, 030601.	7.8	41
21	Diagrammatic expansion for positive spectral functions beyond <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>WApplication to vertex corrections in the electron gas. Physical Review B, 2014, 90, .</mml:mi></mml:mrow></mml:math 	mi> ⊲n aml:r	mrowo
22	Real-time observation of a correlation-driven sub 3 fs charge migration in ionised adenine. Communications Chemistry, 2021, 4, .	4.5	38
23	Nonequilibrium Bethe-Salpeter equation for transient photoabsorption spectroscopy. Physical Review B, 2015, 92, .	3.2	37
24	Some exact properties of the nonequilibrium response function for transient photoabsorption. Physical Review A, 2015, 91, .	2.5	37
25	Charge Separation in Donor–C ₆₀ Complexes with Real-Time Green Functions: The Importance of Nonlocal Correlations. Nano Letters, 2018, 18, 785-792.	9.1	37
26	Spin-flip scattering in time-dependent transport through a quantum dot: Enhanced spin-current and inverse tunneling magnetoresistance. Physical Review B, 2008, 78, .	3.2	36
27	Bound states in time-dependent quantum transport: oscillations and memory effects in current and density. Physical Chemistry Chemical Physics, 2009, 11, 4535.	2.8	36
28	Ultrafast Charge Migration in XUV Photoexcited Phenylalanine: A First-Principles Study Based on Real-Time Nonequilibrium Green's Functions. Journal of Physical Chemistry Letters, 2018, 9, 1353-1358.	4.6	36
29	Image charge dynamics in time-dependent quantum transport. Physical Review B, 2012, 85, .	3.2	35
30	Observation of an Excitonic Mott Transition Through Ultrafast Core- <i>cum</i> -Conduction Photoemission Spectroscopy. Physical Review Letters, 2020, 125, 096401.	7.8	35
31	Fast Green's Function Method for Ultrafast Electron-Boson Dynamics. Physical Review Letters, 2021, 127, 036402.	7.8	35
32	Correlation-Induced Memory Effects in Transport Properties of Low-Dimensional Systems. Physical Review Letters, 2010, 105, 156802.	7.8	33
33	CHEERS: a tool for correlated hole-electron evolution from real-time simulations. Journal of Physics Condensed Matter, 2018, 30, 465901.	1.8	32
34	Pump-driven normal-to-excitonic insulator transition: Josephson oscillations and signatures of BEC-BCS crossover in time-resolved ARPES. Physical Review Materials, 2019, 3, .	2.4	30
35	The role of bound states in time-dependent quantum transport. Applied Physics A: Materials Science and Processing, 2008, 93, 355-364.	2.3	29
36	On the thermalization of a Luttinger liquid after a sequence of sudden interaction quenches. Europhysics Letters, 2011, 95, 10006.	2.0	29

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37	The generalized Kadanoff-Baym ansatz with initial correlations. Physical Review B, 2018, 98, .	3.2	28
38	Kadanoff-Baym approach to time-dependent quantum transport in AC and DC fields. Journal of Physics: Conference Series, 2010, 220, 012017.	0.4	26
39	Assessing the accuracy of Kohn-Sham conductances using the Friedel sum rule. Physical Review B, 2010, 81, .	3.2	25
40	Molecular junctions and molecular motors: Including Coulomb repulsion in electronic friction using nonequilibrium Green's functions. Physical Review B, 2018, 98, .	3.2	25
41	Wick theorem for general initial states. Physical Review B, 2012, 85, .	3.2	24
42	Nonequilibrium Anderson model made simple with density functional theory. Physical Review B, 2016, 94, .	3.2	24
43	Phononic heat transport in the transient regime: An analytic solution. Physical Review B, 2016, 93, .	3.2	24
44	Real-Time <mml:math <br="" xmlns:mml="http://www.w3.org/1998/Math/MathML">display="inline"><mml:mi>G</mml:mi><mml:mi>W</mml:mi> : Toward an <i>AbÂlnitio</i> Description of the Ultrafast Carrier and Exciton Dynamics in Two-Dimensional Materials. Physical Review Letters, 2022, 128, 016801.</mml:math>	7.8	24
45	Time-dependent Landauer–Büttiker formula for transient dynamics. Journal of Physics: Conference Series, 2013, 427, 012014.	0.4	23
46	Transport through correlated systems with density functional theory. Journal of Physics Condensed Matter, 2017, 29, 413002.	1.8	23
47	Real-time dynamics of Auger wave packets and decays in ultrafast charge migration processes. Physical Review A, 2018, 97, .	2.5	22
48	Diagrammatic expansion for positive density-response spectra: Application to the electron gas. Physical Review B, 2015, 91, .	3.2	21
49	An ab-initio approach to describe coherent and non-coherent exciton dynamics. European Physical Journal B, 2018, 91, 1.	1.5	21
50	Ultrafast Quantum Interference in the Charge Migration of Tryptophan. Journal of Physical Chemistry Letters, 2020, 11, 891-899.	4.6	21
51	Dynamically screened vertex correction to <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"> <mml:mrow> <mml:mi>G</mml:mi> <mml:mi>WPhysical Review B, 2020, 102, .</mml:mi></mml:mrow></mml:math 	>¢¢naml:m	ıro ₂o
52	Ultrafast manipulation of electron spins in a double quantum dot device: A real-time numerical and analytical study. Physical Review B, 2008, 78, .	3.2	19
53	Image charge effects in the nonequilibrium Anderson-Holstein model. Physical Review B, 2013, 88, .	3.2	19
54	Distinguishing Majorana zero modes from impurity states through time-resolved transport. New Journal of Physics, 2019, 21, 103038.	2.9	19

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55	Time-resolved ARPES spectra of nonequilibrium excitonic insulators: Revealing macroscopic coherence with ultrashort pulses. Physical Review B, 2020, 101, .	3.2	19
56	Vertex Corrections for Positive-Definite Spectral Functions of Simple Metals. Physical Review Letters, 2016, 117, 206402.	7.8	18
57	Photoinduced dynamics of organic molecules using nonequilibrium Green's functions with second-Born, <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"> <mml:mrow> <mml:mi>G</mml:mi><mml:mi>W<td>ni><ʔiħml:</td><td>mro¹⁸><mmla< td=""></mmla<></td></mml:mi></mml:mrow></mml:math>	ni><ʔiħml:	mro ¹⁸ > <mmla< td=""></mmla<>
58	First-Principles Nonequilibrium Green's Function Approach to Ultrafast Charge Migration in Glycine. Journal of Chemical Theory and Computation, 2019, 15, 4526-4534.	5.3	17
59	Floquet Topological Phase of Nondriven <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>p</mml:mi> -Wave Nonequilibrium Excitonic Insulators. Physical Review Letters, 2020, 125, 106401.</mml:math 	7.8	17
60	Ensemble Density Functional Theory: Insight from the Fluctuation-Dissipation Theorem. Physical Review Letters, 2020, 125, 233001.	7.8	17
61	Time-dependent bond-current functional theory for lattice Hamiltonians: Fundamental theorem and application to electron transport. Chemical Physics, 2011, 391, 164-172.	1.9	15
62	Density functional theory of the Seebeck coefficient in the Coulomb blockade regime. Physical Review B, 2016, 94, .	3.2	14
63	Kondo effect in the Kohn–Sham conductance of multipleâ€level quantum dots. Physica Status Solidi (B): Basic Research, 2013, 250, 2378-2385.	1.5	13
64	Electronic transport in molecular junctions: The generalized Kadanoff–Baym ansatz with initial contact and correlations. Journal of Chemical Physics, 2021, 154, 094104.	3.0	13
65	"W = 0―pairing in Cu-O clusters and in the plane. European Physical Journal B, 1999, 10, 293-304.	1.5	12
66	The Potential of EuPRAXIA@SPARC_LAB for Radiation Based Techniques. Condensed Matter, 2019, 4, 30.	1.8	12
67	Time-linear scaling nonequilibrium Green's function methods for real-time simulations of interacting electrons and bosons. I. Formalism. Physical Review B, 2022, 105, .	3.2	12
68	Canonical transformation of the three-band Hubbard model and hole pairing. Solid State Communications, 1998, 109, 229-233.	1.9	11
69	W=Opairing in(N,N)carbon nanotubes away from half filling. Physical Review B, 2002, 66, .	3.2	11
70	Time-dependent Landauer—Büttiker formalism for superconducting junctions at arbitrary temperatures. Journal of Physics: Conference Series, 2016, 696, 012016.	0.4	11
71	Missing derivative discontinuity of the exchange-correlation energy for attractive interactions: The charge Kondo effect. Physical Review B, 2012, 86, .	3.2	10
72	Time-dependent i-DFT exchange-correlation potentials with memory: applications to the out-of-equilibrium Anderson model. European Physical Journal B, 2018, 91, 1.	1.5	10

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73	Time-linear scaling nonequilibrium Green's function method for real-time simulations of interacting electrons and bosons. II. Dynamics of polarons and doublons. Physical Review B, 2022, 105, .	3.2	10
74	Ultra-nonlocality in density functional theory for photo-emission spectroscopy. Journal of Chemical Physics, 2014, 140, 18A526.	3.0	9
75	Time-resolved photoabsorption in finite systems: A first-principles NEGF approach. Journal of Physics: Conference Series, 2016, 696, 012004.	0.4	9
76	Nonequilibrium spectral functions from multiterminal steady-state density functional theory. Physical Review B, 2019, 100, .	3.2	8
77	Nonadiabatic Van der Pol oscillations in molecular transport. European Physical Journal B, 2014, 87, 1.	1.5	7
78	Transient dynamics in the Anderson–Holstein model with interfacial screening. Journal of Computational Electronics, 2015, 14, 352-359.	2.5	7
79	Benchmarking nonequilibrium Green's functions against configuration interaction for time-dependent Auger decay processes. European Physical Journal B, 2018, 91, 1.	1.5	7
80	Mott Metal-Insulator Transition from Steady-State Density Functional Theory. Physical Review Letters, 2020, 125, 216401.	7.8	7
81	Self-consistent screening enhances the stability of the nonequilibrium excitonic insulator phase. Physical Review B, 2020, 102, .	3.2	7
82	Thermoelectric transport within density functional theory. Physical Review B, 2021, 104, .	3.2	7
83	On-site repulsion as the source of pairing in carbon nanotubes and intercalated graphite. European Physical Journal B, 2002, 30, 139-142.	1.5	6
84	From carriers and virtual excitons to exciton populations: Insights into time-resolved ARPES spectra from an exactly solvable model. Physical Review B, 2021, 103, .	3.2	6
85	W= 0 pairing in Hubbard and related models of low-dimensional superconductors. Journal of Physics Condensed Matter, 2004, 16, R1387-R1422.	1.8	5
86	The Dissection Algorithm for the Secondâ€Born Selfâ€Energy. Physica Status Solidi (B): Basic Research, 2019, 256, 1800573.	1.5	5
87	CANONICAL TRANSFORMATION OF THE HUBBARD MODEL AND $W = 0$ PAIRING: COMPARISON WITH EXACT DIAGONALIZATION RESULTS. International Journal of Modern Physics B, 2000, 14, 2994-2999.	2.0	4
88	Time-dependent quantum transport with superconducting leads. Journal of Physics: Conference Series, 2010, 220, 012012.	0.4	4
89	AC transport in correlated quantum dots: From Kondo to Coulomb blockade regime. Physical Review B, 2018, 97, .	3.2	4
90	Coherence and de-coherence in the Time-Resolved ARPES of realistic materials: An ab-initio perspective. Journal of Electron Spectroscopy and Related Phenomena, 2022, 257, 147189.	1.7	4

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91	Exact ground state of the two-dimensional Hubbard model at half-filling for U=0+. Solid State Communications, 2001, 117, 451-454.	1.9	3
92	Ultrafast creation and melting of nonequilibrium excitonic condensates in bulk WSe2. Physical Review B, 2021, 103, .	3.2	3
93	ÂSpin-disentangled exact diagonalization of repulsive Hubbard systems: superconducting pair propagation. Journal of Physics Condensed Matter, 2002, 14, L709-L714.	1.8	2
94	On Coster–Kronig line shapes of solids. Journal of Physics Condensed Matter, 2008, 20, 474209.	1.8	2
95	Nonâ€Equilibrium Green's Functions. Physica Status Solidi (B): Basic Research, 2019, 256, 1900335.	1.5	2
96	Ultrafast dynamics of adenine following XUV ionization. JPhys Photonics, 0, , .	4.6	2
97	Antiferromagnetism of the two-dimensional Hubbard model at half-filling: the analytic ground state for weak coupling. Journal of Physics Condensed Matter, 2001, 13, 1279-1294.	1.8	1
98	Initial Correlation Effects in Time-Dependent Transport with One-Dimensional Interacting Leads. Nanoscience and Nanotechnology Letters, 2011, 3, 877-881.	0.4	1
99	Superconducting Pairs in Clusters and in the Cu-O Plane. International Journal of Modern Physics B, 1999, 13, 1195-1200.	2.0	0
100	INTERPLANAR HOPPING OF W = 0 BOUND PAIRS. International Journal of Modern Physics B, 2003, 17, 567-572.	2.0	0
101	Evidence for W=0 pairing in repulsive Hubbard square and hexagonal geometries. Physica C: Superconductivity and Its Applications, 2004, 408-410, 236-237.	1.2	0
102	Circulating Currents and Magnetic Moments in Quantum Rings. Nanoscience and Nanotechnology Letters, 2011, 3, 902-906.	0.4	0