Alessandro Sergi

List of Publications by Year
in descending order

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64 papers	1,040 citations	394421 19 h-index	454955 30 g-index
66 all docs	66 docs citations	66 times ranked	528 citing authors

#	Article	IF	Citations
1	NON-HERMITIAN QUANTUM DYNAMICS OF A TWO-LEVEL SYSTEM AND MODELS OF DISSIPATIVE ENVIRONMENTS. International Journal of Modern Physics B, 2013, 27, 1350163.	2.0	88
2	Simulating quantum dynamics in classical environments. Theoretical Chemistry Accounts, 2003, 110, 49-58.	1.4	60
3	Density Functional Study of the Photoactive Yellow Protein's Chromophore. Journal of Physical Chemistry B, 2001, 105, 4386-4391.	2.6	59
4	Comparison and unification of non-Hermitian and Lindblad approaches with applications to open quantum optical systems. Journal of Modern Optics, 2014, 61, 1298-1308.	1.3	54
5	Non-Hamiltonian equations of motion with a conserved energy. Physical Review E, 2001, 64, 056125.	2.1	53
6	Time correlation functions for non-Hermitian quantum systems. Physical Review A, 2015, 91, .	2.5	48
7	Non-Hamiltonian equilibrium statistical mechanics. Physical Review E, 2003, 67, 021101.	2.1	42
8	Quantum-classical dynamics of nonadiabatic chemical reactions. Journal of Chemical Physics, 2003, 118, 8566-8575.	3.0	38
9	Non-Hamiltonian commutators in quantum mechanics. Physical Review E, 2005, 72, 066125.	2.1	38
10	Quantum entropy of systems described by non-Hermitian Hamiltonians. Journal of Statistical Mechanics: Theory and Experiment, 2016, 2016, 033102.	2.3	30
11	Simulation of superoxide-superoxide dismutase association rate for six natural variants. Comparison with the experimental catalytic rate. The Journal of Physical Chemistry, 1994, 98, 10554-10557.	2.9	28
12	Effective binding force calculation in a dimeric protein by molecular dynamics simulation. Journal of Chemical Physics, 2002, 116, 6329-6338.	3.0	27
13	Dynamics-Function Correlation in Cu, Zn Superoxide Dismutase: A Spectroscopic and Molecular Dynamics Simulation Study. Biophysical Journal, 2001, 80, 2556-2567.	0.5	26
14	Quantum-classical limit of quantum correlation functions. Journal of Chemical Physics, 2004, 121, 7565.	3.0	26
15	Numerical and analytical approach to the quantum dynamics of two coupled spins in bosonic baths. Physical Review A, 2009, 80, .	2.5	24
16	Deterministic constant-temperature dynamics for dissipative quantum systems. Journal of Physics A: Mathematical and Theoretical, 2007, 40, F347-F354.	2.1	23
17	Nonadiabatic reaction rates for dissipative quantum-classical systems. Journal of Chemical Physics, 2003, 119, 12776-12783.	3.0	21
18	Linear Quantum Entropy and Non-Hermitian Hamiltonians. Entropy, 2016, 18, 451.	2.2	20

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19	Generalized bracket formulation of constrained dynamics in phase space. Physical Review E, 2004, 69, 021109.	2.1	19
20	Two-Qubit Entanglement Generation through Non-Hermitian Hamiltonians Induced by Repeated Measurements on an Ancilla. Entropy, 2020, 22, 1184.	2.2	19
21	Freezing of soft-core bosons at zero temperature: A variational theory. Physical Review B, 2018, 98, .	3.2	18
22	Filtering schemes in the quantum-classical Liouville approach to nonadiabatic dynamics. Physical Review E, 2013, 88, 033301.	2.1	16
23	Reversible integrators for basic extended system molecular dynamics. Molecular Physics, 1999, 97, 825-832.	1.7	15
24	Freezing a Single Distal Motion in Dihydrofolate Reductase. Journal of Physical Chemistry B, 2006, 110, 2435-2441.	2.6	15
25	Sampling of quantum dynamics at long time. Physical Review E, 2010, 81, 032101.	2.1	15
26	Quasi-Lie Brackets and the Breaking of Time-Translation Symmetry for Quantum Systems Embedded in Classical Baths. Symmetry, 2018, 10, 518.	2.2	15
27	Phase space flows for non-Hamiltonian systems with constraints. Physical Review E, 2005, 72, 031104.	2.1	14
28	On the geometry and entropy of non-Hamiltonian phase space. Journal of Statistical Mechanics: Theory and Experiment, 2007, 2007, P02013-P02013.	2.3	13
29	Statistical mechanics of quantum-classical systems with holonomic constraints. Journal of Chemical Physics, 2006, 124, 024110.	3.0	12
30	On the configurational temperature NosÃ¨â€“Hoover thermostat. Physica A: Statistical Mechanics and Its Applications, 2016, 461, 19-35.	2.6	12
31	Embedding quantum systems with a non-conserved probability in classical environments. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	11
32	Stochastic simulation of long-time nonadiabatic dynamics. Physica Scripta, 2011, T143, 014024.	2.5	10
33	Non-Equilibrium Molecular Dynamics. , 2005, , 745-761.		10
34	Clusterization of weakly-interacting bosons in one dimension: an analytic study at zero temperature. Journal of Physics A: Mathematical and Theoretical, 2019, 52, 015002.	2.1	9
35	Bulgac-Kusnezov-NosÃ©-Hoover thermostats. Physical Review E, 2010, 81, 036705.	2.1	8
36	Evolution of a Non-Hermitian Quantum Single-Molecule Junction at Constant Temperature. Entropy, 2021, 23, 147.	2.2	8

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37	Matrix Algebras in Non-Hermitian Quantum Mechanics. Communications in Theoretical Physics, 2011, 56, 96-98.	2.5	7
38	Molecular dynamics study of the plastic-crystalline phase transition of tetraphosphorus triselenide. Molecular Physics, 1995, 84, 727-742.	1.7	6
39	Quantum-classical dynamics of wave fields. Journal of Chemical Physics, 2007, 126, 074109.	3.0	6
40	Minimum-density anomaly and spatial ordering of softly repulsive particles in a narrow channel. Soft Matter, 2013, 9, 9876.	2.7	6
41	Communication: Quantum dynamics in classical spin baths. Journal of Chemical Physics, 2013, 139, 031101.	3.0	6
42	Computer simulation of quantum dynamics in a classical spin environment. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	6
43	Quantum dynamics of a plasmonic metamolecule with a time-dependent driving. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	6
44	Structure of phosphorus-selenium glasses: results fromab initiomolecular dynamics simulations. Molecular Physics, 2000, 98, 701-707.	1.7	5
45	NosÃ¨â€“Hoover dynamics in quantum phase space. Journal of Physics A: Mathematical and Theoretical, 2008, 41, 355304.	2.1	5
46	Nonadiabatic chemical reactions. Computer Physics Communications, 2005, 169, 400-403.	7.5	4
47	Quantum dynamics of a nano-rod under compression. Physics Letters, Section A: General, Atomic and Solid State Physics, 2013, 377, 1047-1051.	2.1	4
48	Proposal of a Computational Approach for Simulating Thermal Bosonic Fields in Phase Space. Physics, 2019, 1, 402-411.	1.4	4
49	On Computational Strategies within Molecular Dynamics Simulation. Physics Essays, 2007, 20, 629-640.	0.4	4
50	First-principles simulation of phosphorus-selenium systems. Chemical Physics Letters, 1996, 259, 301-306.	2.6	3
51	Experimental and Simulative Dissociation of Dimeric Cu,Zn Superoxide Dismutase Doubly Mutated at the Intersubunit Surface. Biophysical Journal, 2005, 88, 2875-2882.	0.5	3
52	Quantum dynamics in classical thermal baths. Computer Physics Communications, 2013, 184, 2474-2477.	7.5	3
53	Quantum dynamics in the partial Wigner picture. Journal of Physics A: Mathematical and Theoretical, 2013, 46, 395305.	2.1	3
54	A variational mean-field study of clusterization in a zero-temperature system of soft-core bosons. EPJ Web of Conferences, 2020, 230, 00008.	0.3	3

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55	Simulating Reactions That Occur Once in a Blue Moon. , 2005, , 1597-1611.		3
56	Non-Hamiltonian Modeling of Squeezing and Thermal Disorder in Driven Oscillators. Journal of Statistical Physics, 2015, 159, 255-273.	1.2	2
57	Symmetry-Induced Emergence of a Pseudo-Qutrit in the Dipolar Coupling of Two Qubits. Entropy, 2022, 24, 223.	2.2	2
58	MOMENTUM SHIFT IN NONADIABATIC DYNAMICS. Modern Physics Letters B, 2011, 25, 1271-1280.	1.9	1
59	Non-Equilibrium Molecular Dynamics. , 2005, , 745-761.		1
60	DECIDE: A Deterministic Mixed Quantum-Classical Dynamics Approach. Applied Sciences (Switzerland), 2022, 12, 7022.	2.5	1
61	Quantum-Classical Wigner-Liouville Equation. Ukrainian Mathematical Journal, 2005, 57, 891-899.	0.5	0
62	Transient behavior of a model fluid under applied shear. Journal of Chemical Physics, 2013, 138, 184501.	3.0	0
63	Simulating Quantum Dynamics in Classical Nanoscale Environments. , 2020, , 515-544.		0
64	Simulating Reactions That Occur Once in a Blue Moon. , 2005, , 1597-1611.		0