Rocco Martinazzo

List of Publications by Year
in descending order

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99 papers	2,546 citations	185998 28 h-index	223531 46 g-index
104 all docs	104 docs citations	104 times ranked	2466 citing authors

#	Article	IF	Citations
1	Lower Bounds for Nonrelativistic Atomic Energies. ACS Physical Chemistry Au, 2022, 2, 23-37.	1.9	14
2	Dissipative tunneling rates through the incorporation of first-principles electronic friction in instanton rate theory. I. Theory. Journal of Chemical Physics, 2022, 156, .	1.2	6
3	Dissipative tunneling rates through the incorporation of first-principles electronic friction in instanton rate theory. II. Benchmarks and applications. Journal of Chemical Physics, 2022, 156, .	1.2	4
4	Quantum Dynamics with Electronic Friction. Physical Review Letters, 2022, 128, .	2.9	7
5	Quantum theory of electronic friction. Physical Review A, 2022, 105, .	1.0	4
6	Lower Bounds for Coulombic Systems. Journal of Chemical Theory and Computation, 2021, 17, 1535-1547.	2.3	5
7	Interaction of Aromatic Molecules with Forsterite: Accuracy of the Periodic DFT-D4 Method. Journal of Physical Chemistry A, 2021, 125, 2770-2781.	1.1	2
8	The Different Story of Ï€ Bonds. Molecules, 2021, 26, 3805.	1.7	2
9	Comparison of an improved self-consistent lower bound theory with Lehmannâ€™s method for low-lying eigenvalues. Scientific Reports, 2021, 11, 23450.	1.6	3
10	Superhydrogenation of pentacene: the reactivity of zigzag-edges. Physical Chemistry Chemical Physics, 2020, 22, 1557-1565.	1.3	20
11	Process Modeling Issues in the Design of a Continuousâ€Flow Process for the Production of Ibuprofen. Chemical Engineering and Technology, 2020, 43, 2557-2566.	0.9	1
12	Benzodithienyl Silanes for Organic Electronics: AIE Solidâ€State Blue Emitters and High Triplet Energy Chargeâ€Transport Materials. Advanced Optical Materials, 2020, 8, 2001018.	3.6	4
13	Effective Enantiodiscrimination in Electroanalysis Based on a New Inherently Chiral 1,1â€²-Binaphthyl Selector Directly Synthesizable in Enantiopure Form. Molecules, 2020, 25, 2175.	1.7	4
14	Self-consistent theory of lower bounds for eigenvalues. Journal of Chemical Physics, 2020, 152, 244110.	1.2	7
15	Lower bounds to eigenvalues of the SchrÃ¶dinger equation by solution of a 90-y challenge. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 16181-16186.	3.3	8
16	Local-in-Time Error in Variational Quantum Dynamics. Physical Review Letters, 2020, 124, 150601.	2.9	19
17	Vibronic coupling models for donor-acceptor aggregates using an effective-mode scheme: Application to mixed Frenkel and charge-transfer excitons in oligothiophene aggregates. Journal of Chemical Physics, 2019, 150, 244114.	1.2	26
18	Kinetic model for the ammoxidation of ethanol to acetonitrile. Chemical Engineering Science, 2019, 207, 862-875.	1.9	8

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19	Identification of stable configurations in the superhydrogenation sequence of polycyclic aromatic hydrocarbon molecules. Monthly Notices of the Royal Astronomical Society, 2019, 486, 5492-5498.	1.6	25
20	To bend or not to bend, the dilemma of multiple bonds. Physical Chemistry Chemical Physics, 2019, 21, 26342-26350.	1.3	8
21	Dual-Route Hydrogenation of the Graphene/Ni Interface. ACS Nano, 2019, 13, 1828-1838.	7.3	8
22	Comment on â€œTheoretical study of the dynamics of atomic hydrogen adsorbed on graphene multilayersâ€. Physical Review B, 2018, 97, .	1.1	8
23	Full quantum dynamical investigation of the Eleyâ€“Rideal reaction forming H2 on a movable graphitic substrate at T = 0 K. Physical Chemistry Chemical Physics, 2018, 20, 977-988.	1.3	3
24	Multi-configurational Ehrenfest simulations of ultrafast nonadiabatic dynamics in a charge-transfer complex. Journal of Chemical Physics, 2018, 149, 244107.	1.2	17
25	Magnetic Moments and Electron Transport through Chromium-Based Antiferromagnetic Nanojunctions. Materials, 2018, 11, 2030.	1.3	3
26	Sticking of atomic hydrogen on graphene. Journal of Physics Condensed Matter, 2018, 30, 283002.	0.7	30
27	A family of solution-processable macrocyclic and open-chain oligothiophenes with atropoisomeric scaffolds: structural and electronic features for potential energy applications. New Journal of Chemistry, 2017, 41, 10009-10019.	1.4	15
28	Process Simulation for the Design and Scale Up of Heterogeneous Catalytic Process: Kinetic Modelling Issues. Catalysts, 2017, 7, 159.	1.6	22
29	Chapter 11 Ultrafast Energy and Charge Transfer in Functional Molecular Nanoscale Aggregates. , 2017, , 407-436.		1
30	Unitary Approaches to Dissipative Quantum Dynamics. , 2016, , .		1
31	Inherently Chiral Spiderâ€Like Oligothiophenes. Chemistry - A European Journal, 2016, 22, 10839-10847.	1.7	25
32	Inherently Chiral Spider-Like Oligothiophenes. Chemistry - A European Journal, 2016, 22, 10685-10685.	1.7	0
33	Note: Caldeira-Leggett model describes dynamics of hydrogen atoms on graphene. Journal of Chemical Physics, 2016, 145, 126101.	1.2	3
34	Hydrogen on silicene: like or unlike graphene?. Physical Chemistry Chemical Physics, 2016, 18, 15654-15666.	1.3	27
35	Classical and quantum dynamics at surfaces: Basic concepts from simple models. International Journal of Quantum Chemistry, 2016, 116, 1575-1602.	1.0	15
36	Atomic-Scale Defects and Impurities in Graphene. , 2016, , 21-37.		0

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37	Exploiting the Photonic Crystal Properties of TiO₂ Nanotube Arrays To Enhance Photocatalytic Hydrogen Production. ACS Catalysis, 2016, 6, 1345-1353.	5.5	117
38	Hydrogen Recombination and Dimer Formation on Graphite from Ab Initio Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2016, 120, 5032-5040.	1.1	10
39	Quantum dynamical investigation of the isotope effect in H₂ formation on graphite at cold collision energies. Physical Chemistry Chemical Physics, 2016, 18, 6607-6617.	1.3	10
40	Quantum dynamics of hydrogen atoms on graphene. II. Sticking. Journal of Chemical Physics, 2015, 143, 124704.	1.2	18
41	Quantum dynamics of hydrogen atoms on graphene. I. System-bath modeling. Journal of Chemical Physics, 2015, 143, 124703.	1.2	18
42	Electron transport in carbon wires in contact with Ag electrodes: a detailed first principles investigation. Physical Chemistry Chemical Physics, 2015, 17, 18413-18425.	1.3	17
43	Hydrogen adsorption on nitrogen and boron doped graphene. Journal of Physics Condensed Matter, 2015, 27, 425502.	0.7	19
44	Vibrational relaxation and decoherence in structured environments: a numerical investigation. Annalen Der Physik, 2015, 527, 556-569.	0.9	10
45	Non-Markovian reduced dynamics of ultrafast charge transfer at an oligothiopheneâ€"fullerene heterojunction. Chemical Physics, 2014, 442, 111-118.	0.9	17
46	Structural and Optical Properties of Inherently Chiral Polythiophenes: A Combined CD-Electrochemistry, Circularly Polarized Luminescence, and TD-DFT Investigation. Journal of Physical Chemistry C, 2014, 118, 16019-16027.	1.5	32
47	Inherently Chiral Macrocyclic Oligothiophenes: Easily Accessible Electrosensitive Cavities with Outstanding Enantioselection Performances. Chemistry - A European Journal, 2014, 20, 15298-15302.	1.7	57
48	Hydrogen-dimer lines and electron waveguides in graphene. Physical Chemistry Chemical Physics, 2014, 16, 17610-17616.	1.3	4
49	Adiabatic Potential Energy Surfaces for the Low-Energy Collisional Dynamics of C⁺(²P) Ions with H₂ Molecules. Journal of Physical Chemistry A, 2014, 118, 6595-6603.	1.1	10
50	Structure and stability of hydrogenated carbon atom vacancies in graphene. Carbon, 2014, 77, 165-174.	5.4	30
51	Inherently Chiral Macrocyclic Oligothiophenes: Easily Accessible Electrosensitive Cavities with Outstanding Enantioselection Performances. Chemistry - A European Journal, 2014, 20, 15261-15261.	1.7	5
52	Hydrogen Recombination on Graphitic Surfaces. Springer Series in Surface Sciences, 2013, , 157-177.	0.3	4
53	Insights into H ₂ formation in space from ab initio molecular dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 6674-6677.	3.3	30
54	Spin coupling around a carbon atom vacancy in graphene. Physical Review B, 2013, 88, .	1.1	34

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55	Reduced and Exact Quantum Dynamics of the Vibrational Relaxation of a Molecular System Interacting with a Finite-Dimensional Bath. Journal of Physical Chemistry A, 2012, 116, 11118-11127.	1.1	18
56	Compact MCTDH Wave Functions for High-Dimensional System-Bath Quantum Dynamics. Journal of Physical Chemistry A, 2012, 116, 11406-11413.	1.1	16
57	Quantum dynamics of ultrafast charge transfer at an oligothiophene-fullerene heterojunction. Journal of Chemical Physics, 2012, 137, 22A540.	1.2	85
58	Non-Markovian reduced dynamics based upon a hierarchical effective-mode representation. Journal of Chemical Physics, 2012, 137, 144107.	1.2	22
59	The Effect of Atomic-Scale Defects on Graphene Electronic Structure. Carbon Nanostructures, 2012, , 137-145.	0.1	1
60	Hierarchical Effective-Mode Approach for Extended Molecular Systems. Progress in Theoretical Chemistry and Physics, 2012, , 269-283.	0.2	3
61	Surface models and reaction barrier in Eleyâ€"Rideal formation of H2 on graphitic surfaces. Physical Chemistry Chemical Physics, 2011, 13, 16680.	1.3	21
62	Conical Intersections Coupled to an Environment. Advanced Series in Physical Chemistry, 2011, , 301-346.	1.5	6
63	Coherent Excitation Transfer Driven by Torsional Dynamics: a Model Hamiltonian for PPV Type Systems. Zeitschrift Fur Physikalische Chemie, 2011, 225, 541-551.	1.4	22
64	Band Engineering in Graphene with Superlattices of Substitutional Defects. Journal of Physical Chemistry C, 2011, 115, 3250-3256.	1.5	82
65	The Effect of Atomic-Scale Defects and Dopants on Graphene Electronic Structure. , 2011, , .		3
66	Communication: Universal Markovian reduction of Brownian particle dynamics. Journal of Chemical Physics, 2011, 134, 011101.	1.2	97
67	Benchmark calculations for dissipative dynamics of a system coupled to an anharmonic bath with the multiconfiguration time-dependent Hartree method. Journal of Chemical Physics, 2011, 134, 094102.	1.2	18
68	Unraveling a Brownian particleâ€™s memory with effective mode chains. Physical Review E, 2011, 84, 030102.	0.8	27
69	A few simple rules governing hydrogenation of graphene dots. Journal of Chemical Physics, 2011, 135, 164701.	1.2	34
70	Generalized CC-TDSCF and LCSA: The system-energy representation. Journal of Chemical Physics, 2011, 134, 014102.	1.2	7
71	Effective spectral densities for system-environment dynamics at conical intersections: S2â€"S1 conical intersection in pyrazine. Chemical Physics, 2010, 377, 21-29.	0.9	33
72	Symmetry-induced band-gap opening in graphene superlattices. Physical Review B, 2010, 81, .	1.1	93

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73	Quantum Dynamics of the Eleyâ˜Rideal Hydrogen Formation Reaction on Graphite at Typical Interstellar Cloud Conditions. Journal of Physical Chemistry A, 2009, 113, 14545-14553.	1.1	27
74	Understanding adsorption of hydrogen atoms on graphene. Journal of Chemical Physics, 2009, 130, 054704.	1.2	303
75	Quasi-classical trajectory study of the adiabatic reactions occurring on the two lowest-lying electronic states of the LiH2+ system. Physical Chemistry Chemical Physics, 2008, 10, 5545.	1.3	31
76	Physisorption and Diffusion of Hydrogen Atoms on Graphite from Correlated Calculations on the Hâ˜Coronene Model System. Journal of Physical Chemistry C, 2007, 111, 5825-5829.	1.5	91
77	Chemistry at surfaces: from ab initio structures to quantum dynamics. Theoretical Chemistry Accounts, 2007, 117, 805-825.	0.5	28
78	A local coherent-state approximation to system-bath quantum dynamics. Journal of Chemical Physics, 2006, 125, 194102.	1.2	52
79	Quantum study of Eley-Rideal reaction and collision induced desorption of hydrogen atoms on a graphite surface. II. H-physisorbed case. Journal of Chemical Physics, 2006, 124, 124703.	1.2	32
80	Quantum study of Eley-Rideal reaction and collision induced desorption of hydrogen atoms on a graphite surface. I. H-chemisorbed case. Journal of Chemical Physics, 2006, 124, 124702.	1.2	48
81	Testing wave packet dynamics in computing radiative association cross sections. Journal of Chemical Physics, 2005, 122, 094109.	1.2	7
82	Quantum Effects in an Exoergic, Barrierless Reaction at High Collision Energies. Journal of Physical Chemistry A, 2005, 109, 9379-9383.	1.1	21
83	Hot-atom versus Eleyâ€"Rideal dynamics in hydrogen recombination on Ni(100). I. The single-adsorbate case. Journal of Chemical Physics, 2004, 120, 8761-8771.	1.2	34
84	Potential energy surface, bound states, and rotational inelastic cross sections of the He-CH[sub 4] system: A theoretical investigation. Journal of Chemical Physics, 2004, 121, 8261.	1.2	17
85	A modified Variable-Phase algorithm for multichannel scattering with long-range potentials. Computer Physics Communications, 2003, 151, 187-198.	3.0	57
86	Three-dimensional reactive surfaces for the LiH2+ system: an analysis of accurate ab initio results. Chemical Physics, 2003, 287, 335-348.	0.9	39
87	The gas-phase lithium chemistry in the early universe: elementary processes, interaction forces and quantum dynamics. Physics Reports, 2003, 384, 85-119.	10.3	72
88	Accurate potential energy surfaces for the study of lithiumâ€"hydrogen ionic reactions. Journal of Chemical Physics, 2003, 119, 11241-11248.	1.2	67
89	Photoexcitation of LiH2+ from selected initial states: A time-dependent model. Journal of Chemical Physics, 2002, 117, 177-186.	1.2	4
90	Recent developments of the SCVB method. Theoretical and Computational Chemistry, 2002, 10, 261-277.	0.2	16

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91	Reactive Behavior of the [LiH2]+ System II. Collision-Induced Dissociation and Collinear Reaction Dynamics of LiH++H from Quantum Time Dependent Calculations. Journal of Physical Chemistry A, 2001, 105, 10994-11000.	1.1	28
92	Reactive Behavior of the [LiH2]+ System I. Evaluation of the Lower-lying Electronic Potentials for the Collinear Geometries. Journal of Physical Chemistry A, 2001, 105, 10986-10993.	1.1	33
93	Computed orientational anisotropy and vibrational couplings for the LiH + H interaction potential. European Physical Journal D, 2001, 15, 321-329.	0.6	15
94	Possible reaction paths in the LiH+2 chemistry: a computational analysis of the interaction forces. Chemical Physics, 2001, 271, 309-321.	0.9	45
95	A multireference valence bond approach to electronic excited states. Journal of Chemical Physics, 2001, 115, 2917-2925.	1.2	32
96	Testing van der Waals interactions with quantum dynamics: Repulsive anisotropy and well depth in the LiH+He system. Journal of Chemical Physics, 2000, 113, 11071-11078.	1.2	14
97	Applications of a variational coupled-electron pair approach to the calculation of intermolecular interaction in the framework of the VB theory: Study of the van der Waals complex Heâ€"CH4. Journal of Chemical Physics, 2000, 113, 6724-6735.	1.2	13
98	Spatial Energetics of Protonated LiH: Lower-Lying Potential Energy Surfaces from Valence Bond Calculations. Journal of Physical Chemistry A, 2000, 104, 11972-11982.	1.1	31
99	Signatures of coherent vibronic exciton dynamics and conformational control in the two-dimensional electronic spectroscopy of conjugated polymers. Faraday Discussions, 0, 237, 148-167.	1.6	3