Rocco Martinazzo

List of Publications by Citations

95 papers	2,204 citations	27 h-index	43 g-index
104 ext. papers	2,366 ext. citations	4.2 avg, IF	5.08 L-index

#	Paper	IF	Citations
95	Understanding adsorption of hydrogen atoms on graphene. *Journal of Chemical Physics*, **2009**, 130, 054704	3.9	277
94	Exploiting the Photonic Crystal Properties of TiO2 Nanotube Arrays To Enhance Photocatalytic Hydrogen Production. *ACS Catalysis*, **2016**, 6, 1345-1353	13.1	97
93	Symmetry-induced band-gap opening in graphene superlattices. *Physical Review B*, **2010**, 81,	3.3	87
92	Physisorption and Diffusion of Hydrogen Atoms on Graphite from Correlated Calculations on the H□coronene Model System. *Journal of Physical Chemistry C*, **2007**, 111, 5825-5829	3.8	85
91	Communication: Universal Markovian reduction of Brownian particle dynamics. *Journal of Chemical Physics*, **2011**, 134, 011101	3.9	84
90	Quantum dynamics of ultrafast charge transfer at an oligothiophene-fullerene heterojunction. *Journal of Chemical Physics*, **2012**, 137, 22A540	3.9	80
89	Band Engineering in Graphene with Superlattices of Substitutional Defects. *Journal of Physical Chemistry C*, **2011**, 115, 3250-3256	3.8	76
88	The gas-phase lithium chemistry in the early universe: elementary processes, interaction forces and quantum dynamics. *Physics Reports*, **2003**, 384, 85-119	27.7	66
87	Accurate potential energy surfaces for the study of lithium□hydrogen ionic reactions. *Journal of Chemical Physics*, **2003**, 119, 11241-11248	3.9	61
86	A modified Variable-Phase algorithm for multichannel scattering with long-range potentials. *Computer Physics Communications*, **2003**, 151, 187-198	4.2	52
85	A local coherent-state approximation to system-bath quantum dynamics. *Journal of Chemical Physics*, **2006**, 125, 194102	3.9	48
84	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	3.9	47
83	Inherently chiral macrocyclic oligothiophenes: easily accessible electrosensitive cavities with outstanding enantioselection performances. *Chemistry - A European Journal*, **2014**, 20, 15298-302	4.8	46
82	Possible reaction paths in the LiH+2 chemistry: a computational analysis of the interaction forces. *Chemical Physics*, **2001**, 271, 309-321	2.3	42
81	Three-dimensional reactive surfaces for the LiH2+ system: an analysis of accurate ab initio results. *Chemical Physics*, **2003**, 287, 335-348	2.3	36
80	Hot-atom versus Eley-Rideal dynamics in hydrogen recombination on Ni(100). I. The single-adsorbate case. *Journal of Chemical Physics*, **2004**, 120, 8761-71	3.9	33
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	3.9	32

78	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	3.8	31
77	Spatial Energetics of Protonated LiH: Lower-Lying Potential Energy Surfaces from Valence Bond Calculations. *Journal of Physical Chemistry A*, **2000**, 104, 11972-11982	2.8	30
76	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	2.8	30
75	A few simple rules governing hydrogenation of graphene dots. *Journal of Chemical Physics*, **2011**, 135, 164701	3.9	29
74	Spin coupling around a carbon atom vacancy in graphene. *Physical Review B*, **2013**, 88,	3.3	28
73	Effective spectral densities for system-environment dynamics at conical intersections: S2S1 conical intersection in pyrazine. *Chemical Physics*, **2010**, 377, 21-29	2.3	28
72	Chemistry at surfaces: from ab initio structures to quantum dynamics. *Theoretical Chemistry Accounts*, **2007**, 117, 805-825	1.9	28
71	A multireference valence bond approach to electronic excited states. *Journal of Chemical Physics*, **2001**, 115, 2917-2925	3.9	28
70	Insights into H2 formation in space from ab initio molecular dynamics. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 6674-7	11.5	27
69	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	2.8	27
68	Structure and stability of hydrogenated carbon atom vacancies in graphene. *Carbon*, **2014**, 77, 165-174	10.4	26
67	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, 5545-51	3.6	26
66	Unraveling a Brownian particle's memory with effective mode chains. *Physical Review E*, **2011**, 84, 030102	2.4	25
65	Quantum dynamics of the Eley-Rideal hydrogen formation reaction on graphite at typical interstellar cloud conditions. *Journal of Physical Chemistry A*, **2009**, 113, 14545-53	2.8	24
64	Inherently Chiral Spider-Like Oligothiophenes. *Chemistry - A European Journal*, **2016**, 22, 10839-47	4.8	22
63	Hydrogen on silicene: like or unlike graphene?. *Physical Chemistry Chemical Physics*, **2016**, 18, 15654-66	3.6	22
62	Sticking of atomic hydrogen on graphene. *Journal of Physics Condensed Matter*, **2018**, 30, 283002	1.8	21
61	Coherent Excitation Transfer Driven by Torsional Dynamics: a Model Hamiltonian for PPV Type Systems. *Zeitschrift Fur Physikalische Chemie*, **2011**, 225, 541-551	3.1	21

60	Quantum effects in an exoergic, barrierless reaction at high collision energies. *Journal of Physical Chemistry A*, **2005**, 109, 9379-83	2.8	20
59	Surface models and reaction barrier in Eley-Rideal formation of H2 on graphitic surfaces. *Physical Chemistry Chemical Physics*, **2011**, 13, 16680-8	3.6	19
58	Process Simulation for the Design and Scale Up of Heterogeneous Catalytic Process: Kinetic Modelling Issues. *Catalysts*, **2017**, 7, 159	4	17
57	Electron transport in carbon wires in contact with Ag electrodes: a detailed first principles investigation. *Physical Chemistry Chemical Physics*, **2015**, 17, 18413-25	3.6	17
56	Non-Markovian reduced dynamics based upon a hierarchical effective-mode representation. *Journal of Chemical Physics*, **2012**, 137, 144107	3.9	17
55	Potential energy surface, bound states, and rotational inelastic cross sections of the He-CH4 system: a theoretical investigation. *Journal of Chemical Physics*, **2004**, 121, 8261-70	3.9	17
54	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	3.9	16
53	Non-Markovian reduced dynamics of ultrafast charge transfer at an oligothiophene–fullerene heterojunction. *Chemical Physics*, **2014**, 442, 111-118	2.3	16
52	Quantum dynamics of hydrogen atoms on graphene. II. Sticking. *Journal of Chemical Physics*, **2015**, 143, 124704	3.9	16
51	Quantum dynamics of hydrogen atoms on graphene. I. System-bath modeling. *Journal of Chemical Physics*, **2015**, 143, 124703	3.9	16
50	Compact MCTDH wave functions for high-dimensional system-bath quantum dynamics. *Journal of Physical Chemistry A*, **2012**, 116, 11406-13	2.8	16
49	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	3.9	16
48	Identification of stable configurations in the superhydrogenation sequence of polycyclic aromatic hydrocarbon molecules. *Monthly Notices of the Royal Astronomical Society*, **2019**, 486, 5492-5498	4.3	15
47	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	3.6	14
46	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, 11118-27	2.8	14
45	Computed orientational anisotropy and vibrational couplings for the LiH + H interaction potential. *European Physical Journal D*, **2001**, 15, 321-329	1.3	14
44	Hydrogen adsorption on nitrogen and boron doped graphene. *Journal of Physics Condensed Matter*, **2015**, 27, 425502	1.8	13
43	Recent developments of the SCVB method. *Theoretical and Computational Chemistry*, **2002**, 10, 261-277		13

42	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	3.9	13
41	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 He□CH4. *Journal of Chemical Physics*, **2000**, 113, 6724-6735	3.9	11
40	Multi-configurational Ehrenfest simulations of ultrafast nonadiabatic dynamics in a charge-transfer complex. *Journal of Chemical Physics*, **2018**, 149, 244107	3.9	11
39	Hydrogen Recombination and Dimer Formation on Graphite from Ab Initio Molecular Dynamics Simulations. *Journal of Physical Chemistry A*, **2016**, 120, 5032-40	2.8	10
38	Classical and quantum dynamics at surfaces: Basic concepts from simple models. *International Journal of Quantum Chemistry*, **2016**, 116, 1575-1602	2.1	10
37	Vibrational relaxation and decoherence in structured environments: a numerical investigation. *Annalen Der Physik*, **2015**, 527, 556-569	2.6	9
36	Quantum dynamical investigation of the isotope effect in H2 formation on graphite at cold collision energies. *Physical Chemistry Chemical Physics*, **2016**, 18, 6607-17	3.6	9
35	Superhydrogenation of pentacene: the reactivity of zigzag-edges. *Physical Chemistry Chemical Physics*, **2020**, 22, 1557-1565	3.6	9
34	Adiabatic potential energy surfaces for the low-energy collisional dynamics of C(+)((2)P) ions with H2 molecules. *Journal of Physical Chemistry A*, **2014**, 118, 6595-603	2.8	8
33	Testing wave packet dynamics in computing radiative association cross sections. *Journal of Chemical Physics*, **2005**, 122, 094109	3.9	7
32	To bend or not to bend, the dilemma of multiple bonds. *Physical Chemistry Chemical Physics*, **2019**, 21, 26342-26350	3.6	7
31	Dual-Route Hydrogenation of the Graphene/Ni Interface. *ACS Nano*, **2019**, 13, 1828-1838	16.7	7
30	Self-consistent theory of lower bounds for eigenvalues. *Journal of Chemical Physics*, **2020**, 152, 244110	3.9	6
29	Comment on □heoretical study of the dynamics of atomic hydrogen adsorbed on graphene multilayers□*Physical Review B*, **2018**, 97,	3.3	6
28	Lower bounds to eigenvalues of the Schr□inger 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	11.5	5
27	Inherently Chiral Macrocyclic Oligothiophenes: Easily Accessible Electrosensitive Cavities with Outstanding Enantioselection Performances. *Chemistry - A European Journal*, **2014**, 20, 15261-15261	4.8	5
26	Conical Intersections Coupled to an Environment. *Advanced Series in Physical Chemistry*, **2011**, 301-346		5
25	Local-in-Time Error in Variational Quantum Dynamics. *Physical Review Letters*, **2020**, 124, 150601	7.4	4

24	Kinetic model for the ammoxidation of ethanol to acetonitrile. *Chemical Engineering Science*, **2019**, 207, 862-875	4.4	4
23	Hydrogen Recombination on Graphitic Surfaces. *Springer Series in Surface Sciences*, **2013**, 157-177	0.4	4
22	Generalized CC-TDSCF and LCSA: The system-energy representation. *Journal of Chemical Physics*, **2011**, 134, 014102	3.9	4
21	Photoexcitation of LiH2+ from selected initial states: A time-dependent model. *Journal of Chemical Physics*, **2002**, 117, 177-186	3.9	4
20	Lower Bounds for Nonrelativistic Atomic Energies.. *ACS Physical Chemistry Au*, **2022**, 2, 23-37		4
19	Hydrogen-dimer lines and electron waveguides in graphene. *Physical Chemistry Chemical Physics*, **2014**, 16, 17610-6	3.6	3
18	Note: Caldeira-Leggett model describes dynamics of hydrogen atoms on graphene. *Journal of Chemical Physics*, **2016**, 145, 126101	3.9	3
17	Lower Bounds for Coulombic Systems. *Journal of Chemical Theory and Computation*, **2021**, 17, 1535-1547	6.4	3
16	Full quantum dynamical investigation of the Eley-Rideal reaction forming H on a movable graphitic substrate at T = 0 K. *Physical Chemistry Chemical Physics*, **2018**, 20, 977-988	3.6	3
15	Effective Enantiodiscrimination in Electroanalysis Based on a New Inherently Chiral 1,1'-binaphthyl Selector Directly Synthesizable in Enantiopure Form. *Molecules*, **2020**, 25,	4.8	2
14	The Effect of Atomic-Scale Defects and Dopants on Graphene Electronic Structure **2011**,		2
13	Hierarchical Effective-Mode Approach for Extended Molecular Systems. *Progress in Theoretical Chemistry and Physics*, **2012**, 269-283	0.6	2
12	Benzodithienyl Silanes for Organic Electronics: AIE Solid-State Blue Emitters and High Triplet Energy Charge-Transport Materials. *Advanced Optical Materials*, **2020**, 8, 2001018	8.1	2
11	Magnetic Moments and Electron Transport through Chromium-Based Antiferromagnetic Nanojunctions. *Materials*, **2018**, 11,	3.5	2
10	Unitary Approaches to Dissipative Quantum Dynamics **2016**,		1
9	Chapter 11 Ultrafast Energy and Charge Transfer in Functional Molecular Nanoscale Aggregates **2017**, 407-436		1
8	The Effect of Atomic-Scale Defects on Graphene Electronic Structure. *Carbon Nanostructures*, **2012**, 137-145	0.6	1
7	Process Modeling Issues in the Design of a Continuous-Flow Process for the Production of Ibuprofen. *Chemical Engineering and Technology*, **2020**, 43, 2557-2566	2	1

6	The Different Story of Bonds. *Molecules*, **2021**, 26,	4.8	1
5	Comparison of an improved self-consistent lower bound theory with Lehmann's method for low-lying eigenvalues. *Scientific Reports*, **2021**, 11, 23450	4.9	1
4	Interaction of Aromatic Molecules with Forsterite: Accuracy of the Periodic DFT-D4 Method. *Journal of Physical Chemistry A*, **2021**, 125, 2770-2781	2.8	0
3	A New Wide Band Gap Form of Hydrogenated Graphene. *Carbon Nanostructures*, **2012**, 33-38	0.6	
2	Inherently Chiral Spider-Like Oligothiophenes. *Chemistry - A European Journal*, **2016**, 22, 10685-10685	4.8	
1	Atomic-Scale Defects and Impurities in Graphene **2016**, 21-37		