# Rocco Martinazzo

List of Publications by Year
in descending order



| 99 | 2,546 | 185998 | 223531 |
|---|---|---|---|
| papers | citations | 28 h-index | 46 g-index |

| 104 | 104 | 104 | 2466 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Understanding adsorption of hydrogen atoms on graphene. Journal of Chemical Physics, 2009, 130, 054704. | 1.2 | 303 |
| 2 | Exploiting the Photonic Crystal Properties of TiO<sub>2</sub> Nanotube Arrays To Enhance Photocatalytic Hydrogen Production. ACS Catalysis, 2016, 6, 1345-1353. | 5.5 | 117 |
| 3 | Communication: Universal Markovian reduction of Brownian particle dynamics. Journal of Chemical Physics, 2011, 134, 011101. | 1.2 | 97 |
| 4 | Symmetry-induced band-gap opening in graphene superlattices. Physical Review B, 2010, 81, . | 1.1 | 93 |
| 5 | 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 |
| 6 | Quantum dynamics of ultrafast charge transfer at an oligothiophene-fullerene heterojunction. Journal of Chemical Physics, 2012, 137, 22A540. | 1.2 | 85 |
| 7 | Band Engineering in Graphene with Superlattices of Substitutional Defects. Journal of Physical Chemistry C, 2011, 115, 3250-3256. | 1.5 | 82 |
| 8 | 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 |
| 9 | Accurate potential energy surfaces for the study of lithiumâ€“hydrogen ionic reactions. Journal of Chemical Physics, 2003, 119, 11241-11248. | 1.2 | 67 |
| 10 | A modified Variable-Phase algorithm for multichannel scattering with long-range potentials. Computer Physics Communications, 2003, 151, 187-198. | 3.0 | 57 |
| 11 | Inherently Chiral Macrocyclic Oligothiophenes: Easily Accessible Electrosensitive Cavities with Outstanding Enantioselection Performances. Chemistry - A European Journal, 2014, 20, 15298-15302. | 1.7 | 57 |
| 12 | A local coherent-state approximation to system-bath quantum dynamics. Journal of Chemical Physics, 2006, 125, 194102. | 1.2 | 52 |
| 13 | 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 |
| 14 | Possible reaction paths in the LiH+2 chemistry: a computational analysis of the interaction forces. Chemical Physics, 2001, 271, 309-321. | 0.9 | 45 |
| 15 | Three-dimensional reactive surfaces for the LiH2+ system: an analysis of accurate ab initio results. Chemical Physics, 2003, 287, 335-348. | 0.9 | 39 |
| 16 | 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 |
| 17 | A few simple rules governing hydrogenation of graphene dots. Journal of Chemical Physics, 2011, 135, 164701. | 1.2 | 34 |
| 18 | Spin coupling around a carbon atom vacancy in graphene. Physical Review B, 2013, 88, . | 1.1 | 34 |

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| 19 | 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 |
| 20 | 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 |
| 21 | A multireference valence bond approach to electronic excited states. Journal of Chemical Physics, 2001, 115, 2917-2925. | 1.2 | 32 |
| 22 | 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 |
| 23 | 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 |
| 24 | 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 |
| 25 | 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 |
| 26 | Insights into H <sub>2</sub> 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 |
| 27 | Structure and stability of hydrogenated carbon atom vacancies in graphene. Carbon, 2014, 77, 165-174. | 5.4 | 30 |
| 28 | Sticking of atomic hydrogen on graphene. Journal of Physics Condensed Matter, 2018, 30, 283002. | 0.7 | 30 |
| 29 | 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 |
| 30 | Chemistry at surfaces: from ab initio structures to quantum dynamics. Theoretical Chemistry Accounts, 2007, 117, 805-825. | 0.5 | 28 |
| 31 | 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 |
| 32 | Unraveling a Brownian particleâ€™s memory with effective mode chains. Physical Review E, 2011, 84, 030102. | 0.8 | 27 |
| 33 | Hydrogen on silicene: like or unlike graphene?. Physical Chemistry Chemical Physics, 2016, 18, 15654-15666. | 1.3 | 27 |
| 34 | 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 |
| 35 | Inherently Chiral Spiderâ€Like Oligothiophenes. Chemistry - A European Journal, 2016, 22, 10839-10847. | 1.7 | 25 |
| 36 | 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 |

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| 37 | 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 |
| 38 | Non-Markovian reduced dynamics based upon a hierarchical effective-mode representation. Journal of Chemical Physics, 2012, 137, 144107. | 1.2 | 22 |
| 39 | Process Simulation for the Design and Scale Up of Heterogeneous Catalytic Process: Kinetic Modelling Issues. Catalysts, 2017, 7, 159. | 1.6 | 22 |
| 40 | Quantum Effects in an Exoergic, Barrierless Reaction at High Collision Energies. Journal of Physical Chemistry A, 2005, 109, 9379-9383. | 1.1 | 21 |
| 41 | Surface models and reaction barrier in Eleyâ€“Rideal formation of H2 on graphitic surfaces. Physical Chemistry Chemical Physics, 2011, 13, 16680. | 1.3 | 21 |
| 42 | Superhydrogenation of pentacene: the reactivity of zigzag-edges. Physical Chemistry Chemical Physics, 2020, 22, 1557-1565. | 1.3 | 20 |
| 43 | Hydrogen adsorption on nitrogen and boron doped graphene. Journal of Physics Condensed Matter, 2015, 27, 425502. | 0.7 | 19 |
| 44 | Local-in-Time Error in Variational Quantum Dynamics. Physical Review Letters, 2020, 124, 150601. | 2.9 | 19 |
| 45 | 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 |
| 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, 11118-11127. | 1.1 | 18 |
| 47 | Quantum dynamics of hydrogen atoms on graphene. II. Sticking. Journal of Chemical Physics, 2015, 143, 124704. | 1.2 | 18 |
| 48 | Quantum dynamics of hydrogen atoms on graphene. I. System-bath modeling. Journal of Chemical Physics, 2015, 143, 124703. | 1.2 | 18 |
| 49 | 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 |
| 50 | Non-Markovian reduced dynamics of ultrafast charge transfer at an oligothiopheneâ€“fullerene heterojunction. Chemical Physics, 2014, 442, 111-118. | 0.9 | 17 |
| 51 | 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 |
| 52 | Multi-configurational Ehrenfest simulations of ultrafast nonadiabatic dynamics in a charge-transfer complex. Journal of Chemical Physics, 2018, 149, 244107. | 1.2 | 17 |
| 53 | Recent developments of the SCVB method. Theoretical and Computational Chemistry, 2002, 10, 261-277. | 0.2 | 16 |
| 54 | Compact MCTDH Wave Functions for High-Dimensional System-Bath Quantum Dynamics. Journal of Physical Chemistry A, 2012, 116, 11406-11413. | 1.1 | 16 |

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| 55 | Computed orientational anisotropy and vibrational couplings for the LiH + H interaction potential. European Physical Journal D, 2001, 15, 321-329. | 0.6 | 15 |
| 56 | Classical and quantum dynamics at surfaces: Basic concepts from simple models. International Journal of Quantum Chemistry, 2016, 116, 1575-1602. | 1.0 | 15 |
| 57 | 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 |
| 58 | 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 |
| 59 | Lower Bounds for Nonrelativistic Atomic Energies. ACS Physical Chemistry Au, 2022, 2, 23-37. | 1.9 | 14 |
| 60 | 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 |
| 61 | Adiabatic Potential Energy Surfaces for the Low-Energy Collisional Dynamics of C<sup>+</sup>(<sup>2</sup>P) Ions with H<sub>2</sub> Molecules. Journal of Physical Chemistry A, 2014, 118, 6595-6603. | 1.1 | 10 |
| 62 | Vibrational relaxation and decoherence in structured environments: a numerical investigation. Annalen Der Physik, 2015, 527, 556-569. | 0.9 | 10 |
| 63 | 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 |
| 64 | Quantum dynamical investigation of the isotope effect in H<sub>2</sub> formation on graphite at cold collision energies. Physical Chemistry Chemical Physics, 2016, 18, 6607-6617. | 1.3 | 10 |
| 65 | Comment on â€œTheoretical study of the dynamics of atomic hydrogen adsorbed on graphene multilayersâ€. Physical Review B, 2018, 97, . | 1.1 | 8 |
| 66 | Kinetic model for the ammoxidation of ethanol to acetonitrile. Chemical Engineering Science, 2019, 207, 862-875. | 1.9 | 8 |
| 67 | To bend or not to bend, the dilemma of multiple bonds. Physical Chemistry Chemical Physics, 2019, 21, 26342-26350. | 1.3 | 8 |
| 68 | Dual-Route Hydrogenation of the Graphene/Ni Interface. ACS Nano, 2019, 13, 1828-1838. | 7.3 | 8 |
| 69 | 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 |
| 70 | Testing wave packet dynamics in computing radiative association cross sections. Journal of Chemical Physics, 2005, 122, 094109. | 1.2 | 7 |
| 71 | Generalized CC-TDSCF and LCSA: The system-energy representation. Journal of Chemical Physics, 2011, 134, 014102. | 1.2 | 7 |
| 72 | Self-consistent theory of lower bounds for eigenvalues. Journal of Chemical Physics, 2020, 152, 244110. | 1.2 | 7 |

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| 73 | Quantum Dynamics with Electronic Friction. Physical Review Letters, 2022, 128, . | 2.9 | 7 |
| 74 | Conical Intersections Coupled to an Environment. Advanced Series in Physical Chemistry, 2011, , 301-346. | 1.5 | 6 |
| 75 | 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 |
| 76 | Inherently Chiral Macrocyclic Oligothiophenes: Easily Accessible Electrosensitive Cavities with Outstanding Enantioselection Performances. Chemistry - A European Journal, 2014, 20, 15261-15261. | 1.7 | 5 |
| 77 | Lower Bounds for Coulombic Systems. Journal of Chemical Theory and Computation, 2021, 17, 1535-1547. | 2.3 | 5 |
| 78 | Photoexcitation of LiH2+ from selected initial states: A time-dependent model. Journal of Chemical Physics, 2002, 117, 177-186. | 1.2 | 4 |
| 79 | Hydrogen Recombination on Graphitic Surfaces. Springer Series in Surface Sciences, 2013, , 157-177. | 0.3 | 4 |
| 80 | Hydrogen-dimer lines and electron waveguides in graphene. Physical Chemistry Chemical Physics, 2014, 16, 17610-17616. | 1.3 | 4 |
| 81 | 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 |
| 82 | 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 |
| 83 | 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 |
| 84 | Quantum theory of electronic friction. Physical Review A, 2022, 105, . | 1.0 | 4 |
| 85 | The Effect of Atomic-Scale Defects and Dopants on Graphene Electronic Structure. , 2011, , . | | 3 |
| 86 | Note: Caldeira-Leggett model describes dynamics of hydrogen atoms on graphene. Journal of Chemical Physics, 2016, 145, 126101. | 1.2 | 3 |
| 87 | 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 |
| 88 | Magnetic Moments and Electron Transport through Chromium-Based Antiferromagnetic Nanojunctions. Materials, 2018, 11, 2030. | 1.3 | 3 |
| 89 | Hierarchical Effective-Mode Approach for Extended Molecular Systems. Progress in Theoretical Chemistry and Physics, 2012, , 269-283. | 0.2 | 3 |
| 90 | 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 |

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| 91 | 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 |
| 92 | 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 |
| 93 | The Different Story of Ï€ Bonds. Molecules, 2021, 26, 3805. | 1.7 | 2 |
| 94 | Unitary Approaches to Dissipative Quantum Dynamics. , 2016, , . | | 1 |
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| 96 | The Effect of Atomic-Scale Defects on Graphene Electronic Structure. Carbon Nanostructures, 2012, , 137-145. | 0.1 | 1 |
| 97 | Chapter 11 Ultrafast Energy and Charge Transfer in Functional Molecular Nanoscale Aggregates. , 2017, , 407-436. | | 1 |
| 98 | Inherently Chiral Spider-Like Oligothiophenes. Chemistry - A European Journal, 2016, 22, 10685-10685. | 1.7 | 0 |
| 99 | Atomic-Scale Defects and Impurities in Graphene. , 2016, , 21-37. | | 0 |