Raffaele Borrelli

List of Publications by Year
in descending order

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66 papers	1,793 citations	236925 25 h-index	302126 39 g-index
69 all docs	69 docs citations	69 times ranked	1253 citing authors

#	Article	IF	Citations
1	Ultrafast carrier dynamics at organic donorâ€“acceptor interfacesâ€”a quantum-based assessment of the hopping model. JPhys Materials, 2022, 5, 024001.	4.2	6
2	Vibronic coherences in light harvesting nanotubes: unravelling the role of dark states. Journal of Materials Chemistry C, 2022, 10, 7216-7226.	5.5	8
3	Hierarchical equations of motion approach to hybrid fermionic and bosonic environments: Matrix product state formulation in twin space. Journal of Chemical Physics, 2022, 156, .	3.0	13
4	Transparent and Colorless Dye-Sensitized Solar Cells Exceeding 75% Average Visible Transmittance. Jacs Au, 2021, 1, 409-426.	7.9	66
5	Hierarchical Equations-of-Motion Method for Momentum Systemâ€“Bath Coupling. Journal of Physical Chemistry B, 2021, 125, 4863-4873.	2.6	2
6	Probing photoinduced proton coupled electron transfer process by means of two-dimensional resonant electronicâ€“vibrational spectroscopy. Journal of Chemical Physics, 2021, 154, 144104.	3.0	6
7	Expanding the Range of Hierarchical Equations of Motion by Tensor-Train Implementation. Journal of Physical Chemistry B, 2021, 125, 5397-5407.	2.6	16
8	Finite temperature quantum dynamics of complex systems: Integrating <scp>thermoâ€field</scp> theories and <scp>tensorâ€train</scp> methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1539.	14.6	35
9	Simulation of Time- and Frequency-Resolved Four-Wave-Mixing Signals at Finite Temperatures: A Thermo-Field Dynamics Approach. Journal of Chemical Theory and Computation, 2021, 17, 4359-4373.	5.3	15
10	Simulation of Nonlinear Femtosecond Signals at Finite Temperature via a Thermo Field Dynamics-Tensor Train Method: General Theory and Application to Time- and Frequency-Resolved Fluorescence of the Fennaâ€“Matthewsâ€“Olson Complex. Journal of Chemical Theory and Computation, 2021, 17, 4316-4331.	5.3	20
11	Efficient quantum dynamics simulations of complex molecular systems: A unified treatment of dynamic and static disorder. Journal of Chemical Physics, 2021, 155, 134102.	3.0	11
12	Reliable Predictions of Benzophenone Singletâ€“Triplet Transition Rates: A Second-Order Cumulant Approach. Journal of Physical Chemistry A, 2021, 125, 43-49.	2.5	3
13	Generalized Huang-Rhys factors for molecular aggregates. Chemical Physics, 2020, 528, 110495.	1.9	14
14	Proton tunneling in a two-dimensional potential energy surface with a non-linear systemâ€“bath interaction: Thermal suppression of reaction rate. Journal of Chemical Physics, 2020, 152, 214114.	3.0	19
15	Quantum dynamics of vibrational energy flow in oscillator chains driven by anharmonic interactions. New Journal of Physics, 2020, 22, 123002.	2.9	7
16	Tunable Redox Potential, Optical Properties, and Enhanced Stability of Modified Ferrocene-Based Complexes. ACS Omega, 2019, 4, 14780-14789.	3.5	71
17	Density matrix dynamics in twin-formulation: An efficient methodology based on tensor-train representation of reduced equations of motion. Journal of Chemical Physics, 2019, 150, 234102.	3.0	35
18	Disentangling Electronic and Vibrational Effects in the Prediction of Band Shapes for Singletâ€“Triplet Transitions. Journal of Physical Chemistry C, 2019, 123, 14173-14179.	3.1	10

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19	Origin of Unexpectedly Simple Oscillatory Responses in the Excited-State Dynamics of Disordered Molecular Aggregates. Journal of Physical Chemistry Letters, 2019, 10, 2806-2810.	4.6	19
20	Transient and Enduring Electronic Resonances Drive Coherent Long Distance Charge Transport in Molecular Wires. Journal of Physical Chemistry Letters, 2019, 10, 1845-1851.	4.6	17
21	Excited state photophysics of squaraine dyes for photovoltaic applications: an alternative deactivation scenario. Journal of Materials Chemistry C, 2018, 6, 2778-2785.	5.5	25
22	Hole Hopping Rates in Organic Semiconductors: A Second-Order Cumulant Approach. Journal of Chemical Theory and Computation, 2018, 14, 1594-1601.	5.3	31
23	Second-Order Cumulant Approach for the Evaluation of Anisotropic Hole Mobility in Organic Semiconductors. Journal of Physical Chemistry C, 2018, 122, 25849-25857.	3.1	29
24	Theoretical study of charge-transfer processes at finite temperature using a novel thermal SchrÃ¶dinger equation. Chemical Physics, 2018, 515, 236-241.	1.9	17
25	Spectroscopic investigation of squaraine dyes. Proceedings of SPIE, 2017, , .	0.8	4
26	Dynamics of Coupled Electronâ€“Boson Systems with the Multiple Davydov D₁ Ansatz and the Generalized Coherent State. Journal of Physical Chemistry A, 2017, 121, 8757-8770.	2.5	32
27	Thermal SchrÃ¶dinger Equation: Efficient Tool for Simulation of Manyâ€Body Quantum Dynamics at Finite Temperature. Annalen Der Physik, 2017, 529, 1700200.	2.4	19
28	Simulation of Quantum Dynamics of Excitonic Systems at Finite Temperature: an efficient method based on Thermo Field Dynamics. Scientific Reports, 2017, 7, 9127.	3.3	50
29	Efficient orientational averaging of nonlinear optical signals in multi-chromophore systems. Journal of Chemical Physics, 2017, 147, 044114.	3.0	13
30	Dicyanovinyl and Cyano-Ester Benzoindolenine Squaraine Dyes: The Effect of the Central Functionalization on Dye-Sensitized Solar Cell Performance. Energies, 2016, 9, 486.	3.1	25
31	Quantum electron-vibrational dynamics at finite temperature: Thermo field dynamics approach. Journal of Chemical Physics, 2016, 145, 224101.	3.0	58
32	Quantum dynamics of electronic transitions with Gauss-Hermite wave packets. Journal of Chemical Physics, 2016, 144, 114102.	3.0	19
33	The Generalized Coherent State ansatz: Application to quantum electron-vibrational dynamics. Chemical Physics, 2016, 481, 91-98.	1.9	13
34	First-Principle Calculations of the Band Shapes of Singletâ€“Triplet Transitions. Journal of Physical Chemistry C, 2016, 120, 24605-24614.	3.1	8
35	Absorption Band Shapes of a Pushâ€–Pull Dye Approaching the Cyanine Limit: A Challenging Case for First Principle Calculations. Journal of Physical Chemistry A, 2016, 120, 5581-5589.	2.5	31
36	Quantum Dynamics of Radiationless Electronic Transitions Including Normal Modes Displacements and Duschinsky Rotations: A Second-Order Cumulant Approach. Journal of Chemical Theory and Computation, 2015, 11, 415-422.	5.3	19

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37	First Principle Analysis of Charge Dissociation and Charge Recombination Processes in Organic Solar Cells. Journal of Physical Chemistry C, 2015, 119, 18870-18876.	3.1	8
38	Vibronic couplings and coherent electron transfer in bridged systems. Physical Chemistry Chemical Physics, 2015, 17, 30937-30945.	2.8	23
39	Theoretical and experimental determination of the absorption and emission spectra of a prototypical indolenine-based squaraine dye. Physical Chemistry Chemical Physics, 2014, 16, 2390-2398.	2.8	28
40	Panchromatic symmetrical squaraines: a step forward in the molecular engineering of low cost blue-greenish sensitizers for dye-sensitized solar cells. Physical Chemistry Chemical Physics, 2014, 16, 24173-24177.	2.8	41
41	Hole hopping rates in single strand oligonucleotides. Chemical Physics, 2014, 440, 25-30.	1.9	15
42	Franckâ€“Condon factorsâ€”Computational approaches and recent developments. Canadian Journal of Chemistry, 2013, 91, 495-504.	1.1	52
43	Computational investigation of the photoinduced homolytic dissociation of water in the pyridineâ€“water complex. Physical Chemistry Chemical Physics, 2013, 15, 5957.	2.8	51
44	Elementary electron transfer reactions: from basic concepts to recent computational advances. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 542-559.	14.6	32
45	Franckâ€“Condon factors in curvilinear coordinates: the photoelectron spectrum of ammonia. Highlights in Theoretical Chemistry, 2013, , 207-216.	0.0	0
46	Quantum dynamics of electron-transfer reactions: photoinduced intermolecular electron transfer in a porphyrinâ€“quinone complex. Molecular Physics, 2012, 110, 751-763.	1.7	25
47	Generating Function Approach to the Calculation of Spectral Band Shapes of Free-Base Chlorin Including Duschinsky and Herzbergâ€“Teller Effects. Journal of Physical Chemistry A, 2012, 116, 9934-9940.	2.5	78
48	Crossing Electronic States in the Franckâ€“Condon Zone of Carbon Dioxide: A Five-Fold Closed Seam of Conical and Glancing Intersections. Journal of Physical Chemistry Letters, 2012, 3, 3223-3227.	4.6	14
49	Franckâ€“Condon factors in curvilinear coordinates: the photoelectron spectrum of ammonia. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	38
50	The temperature dependence of radiationless transition rates from ab initio computations. Physical Chemistry Chemical Physics, 2011, 13, 4420.	2.8	57
51	First-principles study of photoinduced electron-transfer dynamics in a Mgâ€“porphyrinâ€“quinone complex. Chemical Physics Letters, 2010, 498, 230-234.	2.6	22
52	Photoelectron Spectrum of Ammonia, a Test Case for the Calculation of Franckâ^'Condon Factors in Molecules Undergoing Large Geometrical Displacements upon Photoionization. Journal of Physical Chemistry A, 2009, 113, 14831-14837.	2.5	36
53	The electron photodetachment spectrum of c-C4F8â^': A test case for the computation of Franck-Condon factors of highly flexible molecules. Journal of Chemical Physics, 2008, 128, 044303.	3.0	46
54	Perturbative calculation of Franckâ€“Condon integrals: New hints for a rational implementation. Journal of Chemical Physics, 2008, 129, 064116.	3.0	13

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55	Quantum Dynamics of Electron Transfer from Bacteriochlorophyll to Pheophytin in Bacterial Reaction Centers. Journal of Chemical Theory and Computation, 2007, 3, 673-680.	5.3	35
56	Franckâ€“Condon analysis of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si4.gif" display="inline" overflow="scroll"><mml:mrow><mml:msubsup><mml:mrow><mml:mtext>SF</mml:mtext></mml:mrow><mml:mrow><mml:mn>6</mml:mn></mr electron photodetachment spectrum. Chemical Physics Letters, 2007, 445, 84-88.	2.6	9
57	Electron transfer rates and Franckâ€“Condon factors: an application to the early electron transfer steps in photosynthetic reaction centers. Theoretical Chemistry Accounts, 2007, 117, 957-967.	1.4	21
58	The vibrational progressions of the Nâ†'V electronic transition of ethylene: A test case for the computation of Franck-Condon factors of highly flexible photoexcited molecules. Journal of Chemical Physics, 2006, 125, 194308.	3.0	90
59	Catalytic and Radiative Behaviors of ZrB2-SiC Ultrahigh Temperature Ceramic Composites. Journal of Spacecraft and Rockets, 2006, 43, 1004-1012.	1.9	59
60	Intramolecular reorganization energies and Franckâ€“Condon integrals for ET from pheophytin to quinone in bacterial photosynthetic reaction centers. Chemical Physics Letters, 2005, 413, 210-215.	2.6	5
61	Role of Intramolecular Vibrations in Long-Range Electron Transfer between Pheophytin and Ubiquinone in Bacterial Photosynthetic Reaction Centers. Biophysical Journal, 2005, 89, 830-841.	0.5	28
62	Dynamics of radiationless transitions in large molecular systems: A Franckâ€“Condon-based method accounting for displacements and rotations of all the normal coordinates. Journal of Chemical Physics, 2003, 119, 8437-8448.	3.0	123
63	A Simple Method for Estimating Activation Energies of Proton-Transfer Reactionsâ€. Journal of Physical Chemistry A, 2002, 106, 7018-7025.	2.5	6
64	Excited state intramolecular proton transfer in free base hemiporphyrazine. Chemical Physics Letters, 2002, 354, 160-164.	2.6	12
65	The occurrence of electron transfer in aromatic nitration: dynamical aspects. Theoretical Chemistry Accounts, 2000, 104, 218-222.	1.4	14
66	Proton Assisted Electron Transfer. Advances in Quantum Chemistry, 2000, 36, 301-322.	0.8	10