

# 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	Dynamics of radiationless transitions in large molecular systems: A Franck-Condon-based method accounting for displacements and rotations of all the normal coordinates. <i>Journal of Chemical Physics</i> , 2003, 119, 8437-8448.	3.0	123
2	The vibrational progressions of the N $\pi^*$ V electronic transition of ethylene: A test case for the computation of Franck-Condon factors of highly flexible photoexcited molecules. <i>Journal of Chemical Physics</i> , 2006, 125, 194308.	3.0	90
3	Generating Function Approach to the Calculation of Spectral Band Shapes of Free-Base Chlorin Including Duschinsky and Herzberg-Teller Effects. <i>Journal of Physical Chemistry A</i> , 2012, 116, 9934-9940.	2.5	78
4	Tunable Redox Potential, Optical Properties, and Enhanced Stability of Modified Ferrocene-Based Complexes. <i>ACS Omega</i> , 2019, 4, 14780-14789.	3.5	71
5	Transparent and Colorless Dye-Sensitized Solar Cells Exceeding 75% Average Visible Transmittance. <i>Jacs Au</i> , 2021, 1, 409-426.	7.9	66
6	Catalytic and Radiative Behaviors of ZrB <sub>2</sub> -SiC Ultrahigh Temperature Ceramic Composites. <i>Journal of Spacecraft and Rockets</i> , 2006, 43, 1004-1012.	1.9	59
7	Quantum electron-vibrational dynamics at finite temperature: Thermo field dynamics approach. <i>Journal of Chemical Physics</i> , 2016, 145, 224101.	3.0	58
8	The temperature dependence of radiationless transition rates from ab initio computations. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 4420.	2.8	57
9	Franck-Condon factors—Computational approaches and recent developments. <i>Canadian Journal of Chemistry</i> , 2013, 91, 495-504.	1.1	52
10	Computational investigation of the photoinduced homolytic dissociation of water in the pyridine-water complex. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 5957.	2.8	51
11	Simulation of Quantum Dynamics of Excitonic Systems at Finite Temperature: an efficient method based on Thermo Field Dynamics. <i>Scientific Reports</i> , 2017, 7, 9127.	3.3	50
12	The electron photodetachment spectrum of c-C <sub>4</sub> F <sub>8</sub> : A test case for the computation of Franck-Condon factors of highly flexible molecules. <i>Journal of Chemical Physics</i> , 2008, 128, 044303.	3.0	46
13	Panchromatic symmetrical squaraines: a step forward in the molecular engineering of low cost blue-greenish sensitizers for dye-sensitized solar cells. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 24173-24177.	2.8	41
14	Franck-Condon factors in curvilinear coordinates: the photoelectron spectrum of ammonia. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	1.4	38
15	Photoelectron Spectrum of Ammonia, a Test Case for the Calculation of Franck-Condon Factors in Molecules Undergoing Large Geometrical Displacements upon Photoionization. <i>Journal of Physical Chemistry A</i> , 2009, 113, 14831-14837.	2.5	36
16	Quantum Dynamics of Electron Transfer from Bacteriochlorophyll to Pheophytin in Bacterial Reaction Centers. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 673-680.	5.3	35
17	Density matrix dynamics in twin-formulation: An efficient methodology based on tensor-train representation of reduced equations of motion. <i>Journal of Chemical Physics</i> , 2019, 150, 234102.	3.0	35
18	Finite temperature quantum dynamics of complex systems: Integrating thermo-field theories and tensor-train methods. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021, 11, e1539.	14.6	35

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19	Elementary electron transfer reactions: from basic concepts to recent computational advances. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 542-559.	14.6	32
20	Dynamics of Coupled Electron-Boson Systems with the Multiple Davydov $D_{<sub>1</sub>}$ Ansatz and the Generalized Coherent State. Journal of Physical Chemistry A, 2017, 121, 8757-8770.	2.5	32
21	Absorption Band Shapes of a Push-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
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	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
25	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
26	Quantum dynamics of electron-transfer reactions: photoinduced intermolecular electron transfer in a porphyrin-quinone complex. Molecular Physics, 2012, 110, 751-763.	1.7	25
27	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
28	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
29	Vibronic couplings and coherent electron transfer in bridged systems. Physical Chemistry Chemical Physics, 2015, 17, 30937-30945.	2.8	23
30	First-principles study of photoinduced electron-transfer dynamics in a Mg-porphyrin-quinone complex. Chemical Physics Letters, 2010, 498, 230-234.	2.6	22
31	Electron transfer rates and Franck-Condon factors: an application to the early electron transfer steps in photosynthetic reaction centers. Theoretical Chemistry Accounts, 2007, 117, 957-967.	1.4	21
32	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 Fenna-Matthews-Olson Complex. Journal of Chemical Theory and Computation, 2021, 17, 4316-4331.	5.3	20
33	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
34	Quantum dynamics of electronic transitions with Gauss-Hermite wave packets. Journal of Chemical Physics, 2016, 144, 114102.	3.0	19
35	Thermal Schrödinger Equation: Efficient Tool for Simulation of Many-Body Quantum Dynamics at Finite Temperature. Annalen Der Physik, 2017, 529, 1700200.	2.4	19
36	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

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37	Proton tunneling in a two-dimensional potential energy surface with a non-linear systemâ€ˆbath interaction: Thermal suppression of reaction rate. Journal of Chemical Physics, 2020, 152, 214114.	3.0	19
38	Theoretical study of charge-transfer processes at finite temperature using a novel thermal Schrödinger equation. Chemical Physics, 2018, 515, 236-241.	1.9	17
39	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
40	Expanding the Range of Hierarchical Equations of Motion by Tensor-Train Implementation. Journal of Physical Chemistry B, 2021, 125, 5397-5407.	2.6	16
41	Hole hopping rates in single strand oligonucleotides. Chemical Physics, 2014, 440, 25-30.	1.9	15
42	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
43	The occurrence of electron transfer in aromatic nitration: dynamical aspects. Theoretical Chemistry Accounts, 2000, 104, 218-222.	1.4	14
44	Crossing Electronic States in the Franckâ€ˆCondon 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
45	Generalized Huang-Rhys factors for molecular aggregates. Chemical Physics, 2020, 528, 110495.	1.9	14
46	Perturbative calculation of Franckâ€ˆCondon integrals: New hints for a rational implementation. Journal of Chemical Physics, 2008, 129, 064116.	3.0	13
47	The Generalized Coherent State ansatz: Application to quantum electron-vibrational dynamics. Chemical Physics, 2016, 481, 91-98.	1.9	13
48	Efficient orientational averaging of nonlinear optical signals in multi-chromophore systems. Journal of Chemical Physics, 2017, 147, 044114.	3.0	13
49	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
50	Excited state intramolecular proton transfer in free base hemiporphyrzine. Chemical Physics Letters, 2002, 354, 160-164.	2.6	12
51	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
52	Proton Assisted Electron Transfer. Advances in Quantum Chemistry, 2000, 36, 301-322.	0.8	10
53	Disentangling Electronic and Vibrational Effects in the Prediction of Band Shapes for Singletâ€ˆTriplet Transitions. Journal of Physical Chemistry C, 2019, 123, 14173-14179.	3.1	10
54	Franckâ€ˆCondon analysis of the $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si4.gif" display="inline" overflow="scroll" \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msubsup} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mtext} \rangle \text{SF} \langle \text{mml:mtext} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 6 \langle \text{mml:mrow} \rangle$ electron photodetachment spectrum. Chemical Physics Letters, 2007, 445, 84-88.	2.6	9

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55	First Principle Analysis of Charge Dissociation and Charge Recombination Processes in Organic Solar Cells. <i>Journal of Physical Chemistry C</i> , 2015, 119, 18870-18876.	3.1	8
56	First-Principle Calculations of the Band Shapes of Singletâ€“Triplet Transitions. <i>Journal of Physical Chemistry C</i> , 2016, 120, 24605-24614.	3.1	8
57	Vibronic coherences in light harvesting nanotubes: unravelling the role of dark states. <i>Journal of Materials Chemistry C</i> , 2022, 10, 7216-7226.	5.5	8
58	Quantum dynamics of vibrational energy flow in oscillator chains driven by anharmonic interactions. <i>New Journal of Physics</i> , 2020, 22, 123002.	2.9	7
59	A Simple Method for Estimating Activation Energies of Proton-Transfer Reactionsâ€“. <i>Journal of Physical Chemistry A</i> , 2002, 106, 7018-7025.	2.5	6
60	Probing photoinduced proton coupled electron transfer process by means of two-dimensional resonant electronicâ€“vibrational spectroscopy. <i>Journal of Chemical Physics</i> , 2021, 154, 144104.	3.0	6
61	Ultrafast carrier dynamics at organic donorâ€“acceptor interfacesâ€“a quantum-based assessment of the hopping model. <i>JPhys Materials</i> , 2022, 5, 024001.	4.2	6
62	Intramolecular reorganization energies and Franckâ€“Condon integrals for ET from pheophytin to quinone in bacterial photosynthetic reaction centers. <i>Chemical Physics Letters</i> , 2005, 413, 210-215.	2.6	5
63	Spectroscopic investigation of squaraine dyes. <i>Proceedings of SPIE</i> , 2017, , .	0.8	4
64	Reliable Predictions of Benzophenone Singletâ€“Triplet Transition Rates: A Second-Order Cumulant Approach. <i>Journal of Physical Chemistry A</i> , 2021, 125, 43-49.	2.5	3
65	Hierarchical Equations-of-Motion Method for Momentum Systemâ€“Bath Coupling. <i>Journal of Physical Chemistry B</i> , 2021, 125, 4863-4873.	2.6	2
66	Franckâ€“Condon factors in curvilinear coordinates: the photoelectron spectrum of ammonia. <i>Highlights in Theoretical Chemistry</i> , 2013, , 207-216.	0.0	0