Michele Ceotto

List of Publications by Year
in descending order

71	2,290	159585 30	233421 45
papers	citations	h-index	g-index

74	74	74	1701
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Heavy Atom Tunneling in Organic Reactions at Coupled Cluster Potential Accuracy with a Parallel Implementation of Anharmonic Constant Calculations and Semiclassical Transition State Theory. Journal of Chemical Theory and Computation, 2022, 18, 623-637.	5.3	8
2	Zwitter Ionization of Glycine at Outer Space Conditions due to Microhydration by Six Water Molecules. Physical Review Letters, 2022, 128, 033001.	7.8	7
3	Quantum Vibrational Spectroscopy of Explicitly Solvated Thymidine in Semiclassical Approximation. Journal of Physical Chemistry Letters, 2022, 13, 1350-1355.	4.6	8
4	How many water molecules are needed to solvate one?. Chemical Science, 2021, 12, 2060-2064.	7.4	44
5	Direct measurement and modeling of spontaneous charge migration across anataseâ€“brookite nanoheterojunctions. Journal of Materials Chemistry A, 2021, 9, 7782-7790.	10.3	14
6	Caldeiraâ€“Leggett model vs ab initio potential: A vibrational spectroscopy test of water solvation. Journal of Chemical Physics, 2021, 154, 094106.	3.0	18
7	Thermal and Nuclear Quantum Effects at the Antiferroelectric to Paraelectric Phase Transition in KOH and KOD Crystals. Journal of Physical Chemistry C, 2021, 125, 22328-22334.	3.1	5
8	Unsupervised Machine Learning Neural Gas Algorithm for Accurate Evaluations of the Hessian Matrix in Molecular Dynamics. Journal of Chemical Theory and Computation, 2021, 17, 6733-6746.	5.3	7
9	On-the-fly adiabatically switched semiclassical initial value representation molecular dynamics for vibrational spectroscopy of biomolecules. Journal of Chemical Physics, 2021, 155, 234102.	3.0	13
10	Sensitivity of semiclassical vibrational spectroscopy to potential energy surface accuracy: A test on formaldehyde. Vibrational Spectroscopy, 2020, 106, 103015.	2.2	6
11	Anharmonic quantum nuclear densities from full dimensional vibrational eigenfunctions with application to protonated glycine. Nature Communications, 2020, 11, 4348.	12.8	24
12	Semiclassical Vibrational Spectroscopy of Biological Molecules Using Force Fields. Journal of Chemical Theory and Computation, 2020, 16, 3476-3485.	5.3	18
13	Anharmonic calculations of vibrational spectra for molecular adsorbates: A divide-and-conquer semiclassical molecular dynamics approach. Journal of Chemical Physics, 2020, 152, 104104.	3.0	18
14	Representing molecular ground and excited vibrational eigenstates with nuclear densities obtained from semiclassical initial value representation molecular dynamics. Journal of Chemical Physics, 2020, 153, 214117.	3.0	13
15	Machine learning for vibrational spectroscopy via divide-and-conquer semiclassical initial value representation molecular dynamics with application to N-methylacetamide. Journal of Chemical Physics, 2020, 153, 204104.	3.0	23
16	Semiclassical vibrational spectroscopy with Hessian databases. Journal of Chemical Physics, 2019, 150, 244118.	3.0	25
17	Reduced rovibrational coupling Cartesian dynamics for semiclassical calculations: Application to the spectrum of the Zundel cation. Journal of Chemical Physics, 2019, 151, 114307.	3.0	26
18	Vibrational investigation of nucleobases by means of divide and conquer semiclassical dynamics. Journal of Chemical Physics, 2019, 150, 224107.	3.0	29

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19	An effective semiclassical approach to IR spectroscopy. Journal of Chemical Physics, 2019, 150, 184113.	3.0	29
20	Parallel Implementation of Semiclassical Transition State Theory. Journal of Chemical Theory and Computation, 2019, 15, 2142-2153.	5.3	6
21	Improved semiclassical dynamics through adiabatic switching trajectory sampling. Journal of Chemical Physics, 2019, 151, 214107.	3.0	24
22	Simplified approach to the mixed time-averaging semiclassical initial value representation for the calculation of dense vibrational spectra. Journal of Chemical Physics, 2018, 148, 114107.	3.0	32
23	â€œDivide and conquerâ€•semiclassical molecular dynamics: A practical method for spectroscopic calculations of high dimensional molecular systems. Journal of Chemical Physics, 2018, 148, 014307.	3.0	39
24	â€œDivide-and-conquerâ€•semiclassical molecular dynamics: An application to water clusters. Journal of Chemical Physics, 2018, 148, 104302.	3.0	38
25	A quantum mechanical insight into SN2 reactions: Semiclassical initial value representation calculations of vibrational features of the Clâ^'â‹¯CH3Cl pre-reaction complex with the VENUS suite of codes. Journal of Chemical Physics, 2018, 149, 164113.	3.0	19
26	Protonated glycine supramolecular systems: the need for quantum dynamics. Chemical Science, 2018, 9, 7894-7901.	7.4	35
27	Anharmonic vibrational eigenfunctions and infrared spectra from semiclassical molecular dynamics. Journal of Chemical Physics, 2018, 149, 064115.	3.0	28
28	Herman-Kluk propagator is free from zero-point energy leakage. Chemical Physics, 2018, 515, 231-235.	1.9	27
29	On-the-Fly ab Initio Semiclassical Calculation of Glycine Vibrational Spectrum. Journal of Chemical Theory and Computation, 2017, 13, 2378-2388.	5.3	53
30	A Close Look at the Structure of the TiO₂-APTES Interface in Hybrid Nanomaterials and Its Degradation Pathway: An Experimental and Theoretical Study. Journal of Physical Chemistry C, 2017, 121, 430-440.	3.1	123
31	Atomistic Explanation for Interlayer Charge Transfer in Metalâ€“Semiconductor Nanocomposites: The Case of Silver and Anatase. Journal of Physical Chemistry Letters, 2017, 8, 5372-5377.	4.6	25
32	A quantum method for thermal rate constant calculations from stationary phase approximation of the thermal flux-flux correlation function integral. Journal of Chemical Physics, 2017, 146, 214115.	3.0	10
33	Semiclassical â€œDivide-and-Conquerâ€•Method for Spectroscopic Calculations of High Dimensional Molecular Systems. Physical Review Letters, 2017, 119, 010401.	7.8	57
34	Application of the mixed time-averaging semiclassical initial value representation method to complex molecular spectra. Journal of Chemical Physics, 2017, 147, 164110.	3.0	30
35	The importance of the pre-exponential factor in semiclassical molecular dynamics. Journal of Chemical Physics, 2016, 145, 144107.	3.0	36
36	Mixed semiclassical initial value representation time-averaging propagator for spectroscopic calculations. Journal of Chemical Physics, 2016, 144, 094102.	3.0	40

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37	Kinetics versus thermodynamics in the proline catalyzed aldol reaction. Chemical Science, 2016, 7, 5421-5427.	7.4	25
38	An Efficient Computational Approach for the Calculation of the Vibrational Density of States. Journal of Physical Chemistry A, 2016, 120, 4853-4862.	2.5	18
39	Impregnation versus Bulk Synthesis: How the Synthetic Route Affects the Photocatalytic Efficiency of Nb/Ta:N Codoped TiO₂ Nanomaterials. Journal of Physical Chemistry C, 2015, 119, 24104-24115.	3.1	36
40	Second Generation Nitrogen Doped Titania Nanoparticles: A Comprehensive Electronic and Microstructural Picture. Chinese Journal of Chemistry, 2014, 32, 1195-1213.	4.9	20
41	Graphics processing units accelerated semiclassical initial value representation molecular dynamics. Journal of Chemical Physics, 2014, 140, 174109.	3.0	30
42	Role of the Nitrogen Source in Determining Structure and Morphology of N-Doped Nanocrystalline TiO2. Journal of Physical Chemistry C, 2014, 118, 4797-4807.	3.1	33
43	Unraveling the Cooperative Mechanism of Visible-Light Absorption in Bulk N,Nb Codoped TiO₂ Powders of Nanomaterials. Journal of Physical Chemistry C, 2014, 118, 24152-24164.	3.1	47
44	Helium Isotope Enrichment by Resonant Tunneling through Nanoporous Graphene Bilayers. Journal of Physical Chemistry A, 2014, 118, 6457-6465.	2.5	27
45	Towards Efficient Direct Semiclassical Molecular Dynamics for Complex Molecular Systems. , 2014, , .		0
46	Reproducing Deep Tunneling Splittings, Resonances, and Quantum Frequencies in Vibrational Spectra From a Handful of Direct Ab Initio Semiclassical Trajectories. Journal of Physical Chemistry Letters, 2013, 4, 3407-3412.	4.6	45
47	Investigation and optimization of photocurrent transient measurements on nano-TiO2. Journal of Applied Electrochemistry, 2013, 43, 217-225.	2.9	37
48	Deep nuclear resonant tunneling thermal rate constant calculations. International Journal of Quantum Chemistry, 2013, 113, 1722-1734.	2.0	9
49	Wettability of bare and fluorinated silanes: A combined approach based on surface free energy evaluations and dipole moment calculations. Journal of Colloid and Interface Science, 2013, 389, 284-291.	9.4	63
50	Evaluating the Accuracy of Hessian Approximations for Direct Dynamics Simulations. Journal of Chemical Theory and Computation, 2013, 9, 54-64.	5.3	44
51	Accelerated direct semiclassical molecular dynamics using a compact finite difference Hessian scheme. Journal of Chemical Physics, 2013, 138, 054116.	3.0	50
52	Role of Pr on the Semiconductor Properties of Nanotitania. An Experimental and First-Principles Investigation. Journal of Physical Chemistry C, 2012, 116, 23083-23093.	3.1	19
53	Vibration-assisted tunneling: a semiclassical instanton approach. Molecular Physics, 2012, 110, 547-559.	1.7	19
54	About the Nitrogen Location in Nanocrystalline N-Doped TiO₂: Combined DFT and EXAFS Approach. Journal of Physical Chemistry C, 2012, 116, 1764-1771.	3.1	74

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55	Interplay between Chemistry and Texture in Hydrophobic TiO2 Hybrids. Journal of Physical Chemistry C, 2011, 115, 18649-18658.	3.1	33
56	First principles semiclassical calculations of vibrational eigenfunctions. Journal of Chemical Physics, 2011, 134, 234103.	3.0	35
57	Electronic Structure of Pure and N-Doped TiO₂ Nanocrystals by Electrochemical Experiments and First Principles Calculations. Journal of Physical Chemistry C, 2011, 115, 6381-6391.	3.1	118
58	Photocatalytic removal of ethanol and acetaldehyde by N-promoted TiO2 films: The role of the different nitrogen sources. Catalysis Today, 2011, 161, 169-174.	4.4	43
59	Fighting the curse of dimensionality in first-principles semiclassical calculations: Non-local reference states for large number of dimensions. Journal of Chemical Physics, 2011, 135, 214108.	3.0	45
60	Multiple coherent states semiclassical initial value representation spectra calculations of lateral interactions for CO on Cu(100). Journal of Chemical Physics, 2010, 133, 054701.	3.0	35
61	Multiple coherent states for first-principles semiclassical initial value representation molecular dynamics. Journal of Chemical Physics, 2009, 130, 234113.	3.0	82
62	First-principles semiclassical initial value representation molecular dynamics. Physical Chemistry Chemical Physics, 2009, 11, 3861.	2.8	70
63	Accelerated Superposition State Molecular Dynamics for Condensed Phase Systems. Journal of Chemical Theory and Computation, 2008, 4, 560-568.	5.3	6
64	Quantum reaction rate from higher derivatives of the thermal flux-flux autocorrelation function at time zero. Journal of Chemical Physics, 2005, 122, 044109.	3.0	30
65	Test of the quantum instanton approximation for thermal rate constants for some collinear reactions. Journal of Chemical Physics, 2004, 120, 6356-6362.	3.0	35
66	Quantum instanton approximation for thermal rate constants of chemical reactions. Journal of Chemical Physics, 2003, 119, 1329-1342.	3.0	160
67	A reduced-dimensionality quantum model which incorporates the full-dimensional energy of the system: Application to the vibrational predissociation of Cl2â€“Ne2. Journal of Chemical Physics, 2001, 115, 2146-2156.	3.0	11
68	Internal Coordinate Couplings and Symmetry Properties:Â The Search of a Conical Seam in Protonated Oxygen. Journal of Physical Chemistry A, 2001, 105, 5197-5205.	2.5	0
69	Gas-phase proton affinity of ozone: a computational test of the experimental mechanism. Computational and Theoretical Chemistry, 2001, 543, 115-122.	1.5	1
70	Charge-transfer effects in the gas-phase protonation of ozone: Locating the conical intersections. Journal of Chemical Physics, 2000, 112, 5820-5828.	3.0	9
71	Protonated Ozone:Â Structure, Energetics, and Nonadiabatic Effects. Journal of Physical Chemistry A, 1999, 103, 9984-9994.	2.5	10