Dario De Fazio

List of Publications by Year
in descending order

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46 papers	1,575 citations	201674 27 h-index	302126 39 g-index
46 all docs	46 docs citations	46 times ranked	513 citing authors

#	Article	IF	Citations
1	Benchmark Quantum Kinetics at Low Temperatures toward Absolute Zero and Role of Entrance Channel Wells on Tunneling, Virtual States, and Resonances: The F + HD Reaction. Journal of Physical Chemistry A, 2020, 124, 12-20.	2.5	13
2	Non-adiabatic Quantum Dynamics of the Dissociative Charge Transfer He++H2 â†' He+H+H+. Frontiers in Chemistry, 2019, 7, 249.	3.6	7
3	Quantum Dynamics and Kinetics of the F + H2 and F + D2 Reactions at Low and Ultra-Low Temperatures. Frontiers in Chemistry, 2019, 7, 328.	3.6	25
4	Benchmark Quantum Mechanical Calculations of Vibrationally Resolved Cross Sections and Rate Constants on ab Initio Potential Energy Surfaces for the F + HD Reaction: Comparisons with Experiments. Journal of Physical Chemistry A, 2016, 120, 5288-5299.	2.5	17
5	Complex angular momentum theory of state-to-state integral cross sections: resonance effects in the F + HD â†' HF(vâ€² = 3) + D reaction. Physical Chemistry Chemical Physics, 2015, 17, 18577-18589.	2.8	12
6	Complementarity between Quantum and Classical Mechanics in Chemical Modeling. The H + HeH⁺ â†' H₂⁺ + He Reaction: A Rigourous Test for Reaction Dynamics Methods. Journal of Physical Chemistry A, 2015, 119, 12615-12626.	2.5	23
7	The H + HeH⁺ â†' He + H₂⁺ reaction from the ultra-cold regime to the three-body breakup: exact quantum mechanical integral cross sections and rate constants. Physical Chemistry Chemical Physics, 2014, 16, 11662-11672.	2.8	46
8	Theoretical Reaction Kinetics Astride the Transition between Moderate and Deep Tunneling Regimes: The F + HD Case. Journal of Physical Chemistry A, 2014, 118, 6632-6641.	2.5	38
9	Polarization of molecular angular momentum in the chemical reactions Li + HF and F + HD. Journal of Chemical Physics, 2013, 138, 244302.	3.0	9
10	The He + ${m H}_2^+$H2+ â†' HeH+ + H reaction: Ab initio studies of the potential energy surface, benchmark time-independent quantum dynamics in an extended energy range and comparison with experiments. Journal of Chemical Physics, 2012, 137, 244306.	3.0	46
11	Exact activation energies and phenomenological description of quantum tunneling for model potential energy surfaces. The F+H2 reaction at low temperature. Chemical Physics, 2012, 398, 186-191.	1.9	50
12	Vector correlations in the F + HD reaction. Russian Journal of Physical Chemistry B, 2012, 6, 333-340.	1.3	0
13	Exploring the accuracy level of new potential energy surfaces for the F + HD reactions: from exact quantum rate constants to the state-to-state reaction dynamics. Physical Chemistry Chemical Physics, 2011, 13, 8571.	2.8	40
14	Coalescence of metastable states in chemical reactions: double poles of the scattering matrix and exceptional points. Theoretical Chemistry Accounts, 2011, 129, 141-150.	1.4	9
15	Revisiting the potential energy surface for the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" display="inline" overflow="scroll"><mml:mrow><mml:mtext>He</mml:mtext><mml:mo>+</mml:mo><mml:msubsup><mml:mrow><mml:mtext>H</mml:mtext></mml:mrow> Chemical Physics Letters, 2009, 469, 26-30.	2.6	46
16	Guest species trapped inside carbon nanotubes. Chemical Physics Letters, 2009, 473, 146-150.	2.6	33
17	Quantum Stereodynamics for the Two Product Channels of the F + HD Reaction from the Complete Scattering Matrix in the Stereodirected Representation. Journal of Physical Chemistry A, 2009, 113, 14807-14812.	2.5	16
18	Scattering matrix in reactive collision theory: From resonances to rate constants. Computational and Theoretical Chemistry, 2008, 852, 2-10.	1.5	1

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19	Exact state-to-state quantum dynamics of the F+HDâ†'HF(vâ€²=2)+D reaction on model potential energy surfaces. Journal of Chemical Physics, 2008, 129, 064303.	3.0	32
20	Overlapping resonances and Regge oscillations in the state-to-state integral cross sections of the F+H2 reaction. Journal of Chemical Physics, 2007, 126, 121101.	3.0	30
21	The time-delay route to reactive scattering resonances: the case of the F+H‹sub›2‹/sub›â†' HF + H reaction. Physica Scripta, 2007, 76, C21-C27.	2.5	7
22	Interacting resonances in the F+H2 reaction revisited: Complex terms, Riemann surfaces, and angular distributions. Journal of Chemical Physics, 2007, 126, 084305.	3.0	50
23	On the origin of the forward peak and backward oscillations in the F + H2(v = 0) â†' HF(vâ€² = 2) + H reaction. Physical Chemistry Chemical Physics, 2007, 9, 5664.	2.8	40
24	On the Role of Scattering Resonances in the F + HD Reaction Dynamicsâ€. Journal of Physical Chemistry A, 2007, 111, 12538-12549.	2.5	34
25	Exact quantum calculations of the kinetic isotope effect: Cross sections and rate constants for the F+HD reaction and role of tunneling. Journal of Chemical Physics, 2006, 125, 133109.	3.0	43
26	Benchmark rate constants by the hyperquantization algorithm. The F+H2 reaction for various potential energy surfaces: features of the entrance channel and of the transition state, and low temperature reactivity. Chemical Physics, 2005, 308, 237-253.	1.9	69
27	Direct evaluation of the lifetime matrix by the hyperquantization algorithm: Narrow resonances in the F+H2 reaction dynamics and their splitting for nonzero angular momentum. Journal of Chemical Physics, 2005, 123, 054314.	3.0	55
28	Lifetime of reactive scattering resonances: Q-matrix analysis and angular momentum dependence for the F+H2 reaction by the hyperquantization algorithm. Journal of Chemical Physics, 2004, 121, 11675-11690.	3.0	64
29	Quantum stereodynamics of the F+H2â†'HF+H reaction by the stereodirected S-matrix approach. Chemical Physics, 2004, 301, 251-259.	1.9	26
30	Reactivity enhanced by under-barrier tunneling and resonances: the F+H2â†'HF+H reaction. Chemical Physics Letters, 2003, 371, 504-509.	2.6	42
31	Orthogonal polynomials of a discrete variable as expansion basis sets in quantum mechanics: Hyperquantization algorithm. International Journal of Quantum Chemistry, 2003, 93, 91-111.	2.0	40
32	Exact reaction dynamics by the hyperquantization algorithm: integral and differential cross sections for Fâ€‰+â€‰H2, including long-range and spinâ€"orbit effects. Physical Chemistry Chemical Physics, 2002, 4, 401-415.	2.8	72
33	Dynamics on reactive potential energy surfaces: hyperspherical view and signatures of â€˜quantum chaosâ€™. Molecular Physics, 2001, 99, 443-453.	1.7	6
34	Theory of electronically nonadiabatic reactions: Rotational, Coriolis, spin-orbit couplings and the hyperquantization algorithm. International Journal of Quantum Chemistry, 2001, 85, 368-381.	2.0	31
35	The A+BC reaction by the hyperquantization algorithm: the symmetric hyperspherical parametrization for J > 0. Advances in Quantum Chemistry, 2001, , 103-121.	0.8	25
36	The He + H2+ reaction: a dynamical test on potential energy surfaces for a system exhibiting a pronounced resonance pattern. Chemical Physics Letters, 2000, 318, 619-628.	2.6	70

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37	Ab initiodynamics of the He + H⁺₂â†' HeH⁺+H reaction: a new potential energy surface and quantum mechanical cross-sections. Molecular Physics, 2000, 98, 1835-1849.	1.7	73
38	State-to-state three-atom reactive scattering using adiabatic rotation approximations. Physical Chemistry Chemical Physics, 1999, 1, 1165-1172.	2.8	33
39	Probabilities for the F+H2â†'HF+H reaction by the hyperquantization algorithm: alternative sequential diagonalization schemes. Physical Chemistry Chemical Physics, 1999, 1, 1091-1098.	2.8	30
40	Hyperquantization algorithm. I. Theory for triatomic systems. Journal of Chemical Physics, 1998, 109, 3792-3804.	3.0	102
41	Hyperquantization algorithm. II. Implementation for the F+H2 reaction dynamics including open-shell and spin-orbit interactions. Journal of Chemical Physics, 1998, 109, 3805-3818.	3.0	69
42	A semiclassical model of polarisation forces in atomic scattering. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1995, 33, 27-37.	1.0	11
43	Angular and Hyperangular Momentum Coupling Coefficients as Hahn Polynomials. The Journal of Physical Chemistry, 1995, 99, 15694-15698.	2.9	54
44	A semiclassical model for polarization forces in collisions of electrons and positrons with helium atoms. Journal of Physics B: Atomic, Molecular and Optical Physics, 1994, 27, 303-317.	1.5	22
45	Positron scattering from krypton and xenon. Physical Review A, 1994, 50, 4819-4826.	2.5	10
46	On a parameter-free model for treating polarisation forces in positron scattering processes. Hyperfine Interactions, 1994, 89, 281-298.	0.5	4