Dario De Fazio

List of Publications by Year
in descending order

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	Hyperquantization algorithm. I. Theory for triatomic systems. Journal of Chemical Physics, 1998, 109, 3792-3804.	3.0	102
2	*Ab initio* dynamics of the He + $H_2^+ \to HeH^+$ +H reaction: a new potential energy surface and quantum mechanical cross-sections. Molecular Physics, 2000, 98, 1835-1849.	1.7	73
3	Exact reaction dynamics by the hyperquantization algorithm: integral and differential cross sections for F≃+≃H2, including long-range and spin–orbit effects. Physical Chemistry Chemical Physics, 2002, 4, 401-415.	2.8	72
4	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
5	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
6	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
7	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
8	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
9	Angular and Hyperangular Momentum Coupling Coefficients as Hahn Polynomials. The Journal of Physical Chemistry, 1995, 99, 15694-15698.	2.9	54
10	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
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	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:mr Chemical Physics Letters, 2009, 469, 26-30.	2.6	46
13	The He + ${m H}_2^+$H2+ $\to$ 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
14	The H + HeH$^+$ $\to$ 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
15	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
16	Reactivity enhanced by under-barrier tunneling and resonances: the F+H2→HF+H reaction. Chemical Physics Letters, 2003, 371, 504-509.	2.6	42
17	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
18	On the origin of the forward peak and backward oscillations in the F + H2(v = 0) $\to$ HF(v′ = 2) + H reaction. Physical Chemistry Chemical Physics, 2007, 9, 5664.	2.8	40

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19	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
20	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
21	On the Role of Scattering Resonances in the F + HD Reaction Dynamics†. Journal of Physical Chemistry A, 2007, 111, 12538-12549.	2.5	34
22	State-to-state three-atom reactive scattering using adiabatic rotation approximations. Physical Chemistry Chemical Physics, 1999, 1, 1165-1172.	2.8	33
23	Guest species trapped inside carbon nanotubes. Chemical Physics Letters, 2009, 473, 146-150.	2.6	33
24	Exact state-to-state quantum dynamics of the $F+HD \rightarrow HF(v'=2)+D$ reaction on model potential energy surfaces. Journal of Chemical Physics, 2008, 129, 064303.	3.0	32
25	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
26	Probabilities for the $F+H_2 \rightarrow HF+H$ reaction by the hyperquantization algorithm: alternative sequential diagonalization schemes. Physical Chemistry Chemical Physics, 1999, 1, 1091-1098.	2.8	30
27	Overlapping resonances and Regge oscillations in the state-to-state integral cross sections of the $F+H_2$ reaction. Journal of Chemical Physics, 2007, 126, 121101.	3.0	30
28	Quantum stereodynamics of the $F+H_2 \rightarrow HF+H$ reaction by the stereodirected S-matrix approach. Chemical Physics, 2004, 301, 251-259.	1.9	26
29	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
30	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
31	Complementarity between Quantum and Classical Mechanics in Chemical Modeling. The H + HeH$^+$ $\rightarrow$ H$_2^+$ + He Reaction: A Rigorous Test for Reaction Dynamics Methods. Journal of Physical Chemistry A, 2015, 119, 12615-12626.	2.5	23
32	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
33	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
34	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
35	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
36	Complex angular momentum theory of state-to-state integral cross sections: resonance effects in the F + HD $\rightarrow$ HF(v'= 3) + D reaction. Physical Chemistry Chemical Physics, 2015, 17, 18577-18589.	2.8	12

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37	A semiclassical model of polarisation forces in atomic scattering. Zeitschrift Für Physik D-Atoms Molecules and Clusters, 1995, 33, 27-37.	1.0	11
38	Positron scattering from krypton and xenon. Physical Review A, 1994, 50, 4819-4826.	2.5	10
39	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
40	Polarization of molecular angular momentum in the chemical reactions Li + HF and F + HD. Journal of Chemical Physics, 2013, 138, 244302.	3.0	9
41	The time-delay route to reactive scattering resonances: the case of the $F+H_2 \rightarrow$ HF + H reaction. Physica Scripta, 2007, 76, C21-C27.	2.5	7
42	Non-adiabatic Quantum Dynamics of the Dissociative Charge Transfer He++H2 $\rightarrow$ He+H+H+. Frontiers in Chemistry, 2019, 7, 249.	3.6	7
43	Dynamics on reactive potential energy surfaces: hyperspherical view and signatures of 'quantum chaos'. Molecular Physics, 2001, 99, 443-453.	1.7	6
44	On a parameter-free model for treating polarisation forces in positron scattering processes. Hyperfine Interactions, 1994, 89, 281-298.	0.5	4
45	Scattering matrix in reactive collision theory: From resonances to rate constants. Computational and Theoretical Chemistry, 2008, 852, 2-10.	1.5	1
46	Vector correlations in the F + HD reaction. Russian Journal of Physical Chemistry B, 2012, 6, 333-340.	1.3	0