

# Jorge A Morales

## List of Publications by Year in descending order

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28  
papers

311  
citations

759233

12  
h-index

888059

17  
g-index

28  
all docs

28  
docs citations

28  
times ranked

134  
citing authors

#	ARTICLE	IF	CITATIONS
1	On rotational coherent states in molecular quantum dynamics. <i>Journal of Mathematical Physics</i> , 1999, 40, 766-786.	1.1	36
2	Molecular vibrational state distributions in collisions. <i>Chemical Physics Letters</i> , 1995, 233, 392-398.	2.6	29
3	A theoretical investigation on fullerene-like phosphorus clusters. <i>Chemical Physics Letters</i> , 2004, 396, 27-33.	2.6	29
4	Coherent-states dynamics of the $H^+ + C_2H_2$ reaction at $E_{Lab} = 30 eV$ : A complete electron nuclear dynamics investigation. <i>Chemical Physics Letters</i> , 2005, 414, 405-411.	2.6	22
5	The onset of dissociation in the aqueous LiOH clusters: a solvation study with the effective fragment potential model and quantum mechanics methods. <i>Computational and Theoretical Chemistry</i> , 2004, 681, 27-40.	1.5	15
6	Coherent-states dynamics of the $H^+ + HF$ reaction at $E_{Lab} = 30 eV$ : A complete electron nuclear dynamics investigation. <i>Chemical Physics</i> , 2007, 340, 105-119.	1.9	15
7	Time-dependent density-functional theory method in the electron nuclear dynamics framework. <i>Chemical Physics Letters</i> , 2010, 496, 188-195.	2.6	14
8	Dynamics of $H^+ + N_2$ at $E_{Lab} = 30 eV$ . <i>Journal of Chemical Physics</i> , 2011, 134, 224308.	3.0	14
9	Dynamics of $H^+ + CO$ at $E_{Lab} = 30 eV$ . <i>Journal of Chemical Physics</i> , 2012, 136, 054304.	3.0	14
10	$H^+ + NO(v_i=0) \rightarrow H^+ + NO(v_f=0)$ at $E_{Lab} = 30 eV$ with canonical and Morse coherent states. <i>Chemical Physics Letters</i> , 2012, 551, 42-49.	2.6	14
11	Exploring water radiolysis in proton cancer therapy: Time-dependent, non-adiabatic simulations of $H^+ + (H_2O)_1-6$ . <i>PLoS ONE</i> , 2017, 12, e0174456.	2.5	14
12	Dynamics for the dynamic Frank Harris: Exploring $H^+ + CF_4$ at $E_{Lab} = 20$ and $30 eV$ . <i>International Journal of Quantum Chemistry</i> , 2009, 109, 3026-3035.	2.0	13
13	Some Recent Developments in the Simplest-Level Electron Nuclear Dynamics Method. <i>Advances in Quantum Chemistry</i> , 2013, 66, 113-194.	0.8	13
14	Electron Nuclear Dynamics Simulations of Proton Cancer Therapy Reactions: Water Radiolysis and Proton- and Electron-Induced DNA Damage in Computational Prototypes. <i>Cancers</i> , 2018, 10, 136.	3.7	13
15	Valence-Bond/Coherent-States Approach to the Charge Equilibration Model I. Valence-Bond Models for Diatomic Molecules. <i>Journal of Physical Chemistry A</i> , 2009, 113, 6004-6015.	2.5	11
16	Some coherent-states aspects of the electron nuclear dynamics theory: past and present. <i>Molecular Physics</i> , 2010, 108, 3199-3211.	1.7	11
17	Benchmark coupled-cluster $g$ -tensor calculations with full inclusion of the two-particle spin-orbit contributions. <i>Journal of Chemical Physics</i> , 2017, 146, 164104.	3.0	11
18	In honour of N. Yngve Åhrn: surveying proton cancer therapy reactions with Åhrn's electron nuclear dynamics method. Aqueous clusters radiolysis and DNA-base damage by proton collisions. <i>Molecular Physics</i> , 2015, 113, 297-313.	1.7	8

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19	Symmetry-breaking effects on time-dependent dynamics: correct differential cross sections and other properties in $H^+ + C_2H_4$ at $E_{Lab} = 30$ eV. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 5006-5021.	2.8	4
20	Temporally stable rotational coherent states for molecular simulations. I. Spherical and linear rotor cases. <i>Journal of Chemical Physics</i> , 2020, 152, 134112.	3.0	3
21	Structure and photochemistry of a bio-inspired model for photocatalytic H <sub>2</sub> O splitting: Improved calculations of the Sobolewski and Domcke's Chlorophyll-Imidazole-Benzoquinone model complex. <i>Molecular Physics</i> , 2014, 112, 863-867.	1.7	2
22	Electron nuclear dynamics with plane wave basis sets: complete theory and formalism. <i>Theoretical Chemistry Accounts</i> , 2020, 139, 1.	1.4	2
23	Statistical-law formulas for zero- to two-electron-transfer probabilities in proton molecule and proton cancer therapy reactions from electron nuclear dynamics theory. <i>Journal of Chemical Physics</i> , 2021, 155, 124112.	3.0	2
24	New massively parallel linear-response coupled-cluster module in ACES III: application to static polarisabilities of closed-shell molecules and oligomers and of open-shell radicals. <i>Molecular Physics</i> , 0, , 1-15.	1.7	1
25	Non-adiabatic molecular dynamics simulations of non-charge-transfer and charge-transfer scattering in $H^+ + CO_2$ at $E_{Lab}=30$ eV. <i>Chinese Journal of Chemical Physics</i> , 2018, 31, 300-312.	1.3	1
26	Electron nuclear dynamics of $H^+ + CO_2(000) \rightarrow H^+ + CO_2(v_1v_2v_3)$ at $E_{Lab} = 20.5-30$ eV with coherent-states quantum reconstruction procedure. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 19549-19559.	2.8	0
27	Antibiotic resistance in bacteria: Structure of a novel ssDNA metalloenzyme inhibitor. <i>FASEB Journal</i> , 2012, 26, 962.2.	0.5	0
28	Temporally Stable Rotational Coherent States for Molecular Simulations II. Symmetric Rotor Case. <i>Journal of Chemical Physics</i> , 0, , .	3.0	0