Jorge A Morales

List of Publications by Year
in descending order

28	311	759233 12	888059 17
papers	citations	h-index	g-index

28	28	28	134
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Statistical-law formulas for zero- to two-electron-transfer probabilities in protonâ€“molecule and proton cancer therapy reactions from electron nuclear dynamics theory. Journal of Chemical Physics, 2021, 155, 124112.	3.0	2
2	Electron nuclear dynamics of H+ + CO2 (000) â†' H+ + CO2 (v1v2v3) at ELab = 20.5â€“30 eV with coherent-states quantum reconstruction procedure. Physical Chemistry Chemical Physics, 2020, 22, 19549-19559.	2.8	0
3	Temporally stable rotational coherent states for molecular simulations. I. Spherical and linear rotor cases. Journal of Chemical Physics, 2020, 152, 134112.	3.0	3
4	Electron nuclear dynamics with plane wave basis sets: complete theory and formalism. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	2
5	Symmetry-breaking effects on time-dependent dynamics: correct differential cross sections and other properties in H⁺ + C₂H₄ at E_{Lab} = 30 eV. Physical Chemistry Chemical Physics, 2019, 21, 5006-5021.	2.8	4
6	Non-adiabatic molecular dynamics simulations of non-charge-transfer and charge-transfer scattering in H+ +CO2 at ELab=30 eV. Chinese Journal of Chemical Physics, 2018, 31, 300-312.	1.3	1
7	Electron Nuclear Dynamics Simulations of Proton Cancer Therapy Reactions: Water Radiolysis and Proton- and Electron-Induced DNA Damage in Computational Prototypes. Cancers, 2018, 10, 136.	3.7	13
8	Benchmark coupled-cluster g-tensor calculations with full inclusion of the two-particle spin-orbit contributions. Journal of Chemical Physics, 2017, 146, 164104.	3.0	11
9	Exploring water radiolysis in proton cancer therapy: Time-dependent, non-adiabatic simulations of H+ + (H2O)1-6. PLoS ONE, 2017, 12, e0174456.	2.5	14
10	In honour of N. Yngve Ã–hrn: surveying proton cancer therapy reactions with Ã–hrn's electron nuclear dynamics method. Aqueous clusters radiolysis and DNA-base damage byÂprotonÂcollisions. Molecular Physics, 2015, 113, 297-313.	1.7	8
11	Structure and photochemistry of a bio-inspired model for photocatalytic H2O splitting: Improved calculations of the Sobolewski and Domcke's Chlorophyll-Imidazole-Benzoquinone model complex. Molecular Physics, 2014, 112, 863-867.	1.7	2
12	Some Recent Developments in the Simplest-Level Electron Nuclear Dynamics Method. Advances in Quantum Chemistry, 2013, 66, 113-194.	0.8	13
13	Dynamics of H+ + CO at ELab = 30 eV. Journal of Chemical Physics, 2012, 136, 054304.	3.0	14
14	H++NO(vi=0)â†'H++NO(vf=0â€“2) at ELab=30eV with canonical and Morse coherent states. Chemical Physics Letters, 2012, 551, 42-49.	2.6	14
15	Antibiotic resistance in bacteria: Structure of a novel ssâ€ÐNA metalloenzyme inhibitor. FASEB Journal, 2012, 26, 962.2.	0.5	0
16	Dynamics of H+ + N2 at E Lab = 30 eV. Journal of Chemical Physics, 2011, 134, 224308.	3.0	14
17	Time-dependent density-functional theory method in the electron nuclear dynamics framework. Chemical Physics Letters, 2010, 496, 188-195.	2.6	14
18	Some coherent-states aspects of the electron nuclear dynamics theory: past and present. Molecular Physics, 2010, 108, 3199-3211.	1.7	11

#	Article	IF	Citations
19	Dynamics for the dynamic Frank Harris: Exploring H⁺ + CF₄ at E_{lab} = 20 and 30 eV. International Journal of Quantum Chemistry, 2009, 109, 3026-3035.	2.0	13
20	Valence-Bond/Coherent-States Approach to the Charge Equilibration Model I. Valence-Bond Models for Diatomic Molecules. Journal of Physical Chemistry A, 2009, 113, 6004-6015.	2.5	11
21	Coherent-states dynamics of the H++HF reaction at ELab=30eV: A complete electron nuclear dynamics investigation. Chemical Physics, 2007, 340, 105-119.	1.9	15
22	Coherent-states dynamics of the H++C2H2 reaction at ELab=30eV: A complete electron nuclear dynamics investigation. Chemical Physics Letters, 2005, 414, 405-411.	2.6	22
23	The onset of dissociation in the aqueous LiOH clusters: a solvation study with the effective fragment potential model and quantum mechanics methods. Computational and Theoretical Chemistry, 2004, 681, 27-40.	1.5	15
24	A theoretical investigation on fullerene-like phosphorus clusters. Chemical Physics Letters, 2004, 396, 27-33.	2.6	29
25	On rotational coherent states in molecular quantum dynamics. Journal of Mathematical Physics, 1999, 40, 766-786.	1.1	36
26	Molecular vibrational state distributions in collisions. Chemical Physics Letters, 1995, 233, 392-398.	2.6	29
27	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. Molecular Physics, 0, , 1-15.	1.7	1
28	Temporally Stable Rotational Coherent States for Molecular Simulations II. Symmetric Rotor Case. Journal of Chemical Physics, 0, , .	3.0	0