Aude Simon

List of Publications by Year
in descending order

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62	1,553	331670	315739
papers	citations	21	38
		h-index	g-index

63	63	63	1069
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Infrared spectroscopy of the benzylium-like (and tropylium-like) isomers formed in the â€“H dissociative ionization of methylated PAHs. Journal of Molecular Spectroscopy, 2022, 385, 111620.	1.2	9
2	Water Clusters in Interaction with Corannulene in a Rare Gas Matrix: Structures, Stability and IR Spectra. Photochem, 2022, 2, 237-262.	2.2	4
3	Radiative relaxation in isolated large carbon clusters: Vibrational emission versus recurrent fluorescence. Journal of Chemical Physics, 2022, 156, 144305.	3.0	11
4	Impact of Metals on (Star)Dust Chemistry: A Laboratory Astrophysics Approach. Frontiers in Astronomy and Space Sciences, 2021, 8, .	2.8	2
5	The structure of 1,3-butadiene clusters. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	0
6	Electronic excited states of benzene in interaction with water clusters: influence of structure and size. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	4
7	Hydrogenation of C₂₄ Carbon Clusters: Structural Diversity and Energetic Properties. Journal of Physical Chemistry A, 2021, 125, 5273-5288.	2.5	5
8	Infrared Spectroscopy of Chemically Diverse Carbon Clusters: A Data-Driven Approach. Journal of Physical Chemistry A, 2021, 125, 5509-5518.	2.5	6
9	Simulation of Liquids with the Tight-Binding Density-Functional Approach and Improved Atomic Charges. Journal of Physical Chemistry B, 2020, 124, 7421-7432.	2.6	4
10	Photo-processing of astro-PAHs. Journal of Physics: Conference Series, 2020, 1412, 062002.	0.4	12
11	Quantum modeling of the optical spectra of carbon cluster structural families and relation to the interstellar extinction UV bump. Astronomy and Astrophysics, 2020, 634, A62.	5.1	17
12	Density-functional tight-binding: basic concepts and applications to molecules and clusters. Advances in Physics: X, 2020, 5, 1710252.	4.1	53
13	Perturbation of the Surface of Amorphous Solid Water by the Adsorption of Polycyclic Aromatic Hydrocarbons. Journal of Physical Chemistry C, 2020, 124, 2994-3001.	3.1	14
14	Mapping the structural diversity of C₆₀ carbon clusters and their infrared spectra. Astronomy and Astrophysics, 2019, 625, L11.	5.1	19
15	Ultrafast electronic relaxations from the S₃ state of pyrene. Physical Chemistry Chemical Physics, 2019, 21, 14111-14125.	2.8	8
16	Contribution of the density-functional-based tight-binding scheme to the description of water clusters: methods, applications and extension to bulk systems. Molecular Simulation, 2019, 45, 249-268.	2.0	17
17	Theoretical determination of adsorption and ionisation energies of polycyclic aromatic hydrocarbons on water ice. Physical Chemistry Chemical Physics, 2018, 20, 11941-11953.	2.8	24
18	Photochemistry of Fe:H₂O Adducts in Argon Matrixes: A Combined Experimental and Theoretical Study in the Mid-IR and UVâ€“Visible Regions. Journal of Physical Chemistry A, 2018, 122, 529-542.	2.5	3

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19	Identification of the fragment of the 1-methylpyrene cation by mid-IR spectroscopy. Chemical Physics Letters, 2018, 698, 206-210.	2.6	17
20	Adsorption of PAHs on interstellar ice viewed by classical molecular dynamics. Physical Chemistry Chemical Physics, 2018, 20, 8753-8764.	2.8	21
21	Investigating the importance of edge-structure in the loss of H/H2 of PAH cations: The case of dibenzopyrene isomers. International Journal of Mass Spectrometry, 2018, 429, 189-197.	1.5	17
22	Direct Evidence of the Benzylium and Tropylium Cations as the Two Longâ€Lived Isomers of C₇H₇⁺. ChemPhysChem, 2018, 19, 3182-3185.	2.1	20
23	Dissociation of polycyclic aromatic hydrocarbons at high energy: MD/DFTB simulations versus collision experiments. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	16
24	Atomic hydrogen interactions with gas-phase coronene cations: hydrogenation versus fragmentation. Physical Chemistry Chemical Physics, 2018, 20, 22427-22438.	2.8	22
25	PAH chemistry at eV internal energies. 1. H-shifted isomers. Molecular Astrophysics, 2017, 7, 27-36.	1.6	19
26	PAH chemistry at eV internal energies. 2. Ring alteration and dissociation. Molecular Astrophysics, 2017, 7, 37-59.	1.6	17
27	Dissociation of polycyclic aromatic hydrocarbons: molecular dynamics studies. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2017, 375, 20160195.	3.4	35
28	Formation of coronene:water complexes: FTIR study in argon matrices and theoretical characterisation. Physical Chemistry Chemical Physics, 2017, 19, 8516-8529.	2.8	17
29	Theoretical investigation of the solidâ€“liquid phase transition in protonated water clusters. Physical Chemistry Chemical Physics, 2017, 19, 27288-27298.	2.8	11
30	Structural Characterization of Sulfur-Containing Water Clusters Using a Density-Functional Based Tight-Binding Approach. Journal of Physical Chemistry A, 2016, 120, 9089-9100.	2.5	10
31	Phase changes of the water hexamer and octamer in the gas phase and adsorbed on polycyclic aromatic hydrocarbons. Physical Chemistry Chemical Physics, 2015, 17, 17079-17089.	2.8	25
32	Cationic Methyleneâ€“Pyrene Isomers and Isomerization Pathways: Finite Temperature Theoretical Studies. Journal of Physical Chemistry A, 2015, 119, 12845-12854.	2.5	25
33	Water Clusters in an Argon Matrix: Infrared Spectra from Molecular Dynamics Simulations with a Self-Consistent Charge Density Functional-Based Tight Binding/Force-Field Potential. Journal of Physical Chemistry A, 2015, 119, 2449-2467.	2.5	16
34	Electronic Spectroscopy of [FePAH]⁺ Complexes in the Region of the Diffuse Interstellar Bands: Multireference Wave Function Studies on [FeC₆H₆]⁺. Journal of Physical Chemistry A, 2015, 119, 6123-6130.	2.5	4
35	A density functional tight binding/force field approach to the interaction of molecules with rare gas clusters: Application to (C6H6)+/0Arn clusters. Journal of Chemical Physics, 2014, 140, 034301.	3.0	15
36	Conformational dynamics and finite-temperature infrared spectra of the water octamer adsorbed on coronene. Computational and Theoretical Chemistry, 2013, 1021, 54-61.	2.5	20

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37	Water clusters adsorbed on polycyclic aromatic hydrocarbons: Energetics and conformational dynamics. Journal of Chemical Physics, 2013, 138, 194309.	3.0	27
38	A Novel Approach to the Detection and Characterization of PAH Cations and PAH-Photoproducts. Proceedings of the International Astronomical Union, 2013, 9, 286-290.	0.0	4
39	Vibrational spectroscopy and molecular dynamics of water monomers and dimers adsorbed on polycyclic aromatic hydrocarbons. Physical Chemistry Chemical Physics, 2012, 14, 6771.	2.8	32
40	Extensions of DFTB to investigate molecular complexes and clusters. Physica Status Solidi (B): Basic Research, 2012, 249, 245-258.	1.5	30
41	Molecular dynamics simulations on [FePAH]+Ï€-complexes of astrophysical interest: anharmonic infrared spectroscopy. Physical Chemistry Chemical Physics, 2011, 13, 3359.	2.8	28
42	Perspectives from Quantum Chemistry for molecules and nanograins with astrophysical Interest. EPJ Web of Conferences, 2011, 18, 06003.	0.3	0
43	PAH-related Very Small Grains in photodissociation regions: implications from molecular simulations. EAS Publications Series, 2011, 46, 223-234.	0.3	0
44	[FePAH]⁺complexes and [Fe_xPAH_y]⁺clusters in the interstellar medium: stability and spectroscopy. EAS Publications Series, 2011, 46, 441-446.	0.3	2
45	THE COMPUTED INFRARED SPECTRA OF A VARIETY OF [FePAH]⁺COMPLEXES: MID- AND FAR-INFRARED FEATURES. Astrophysical Journal, 2010, 712, 69-77.	4.5	27
46	Molecular Dynamics Simulations of Anharmonic Infrared Spectra of [SiPAH]⁺Ï€-Complexes. Journal of Physical Chemistry A, 2010, 114, 5846-5854.	2.5	36
47	Signature of [SiPAH]⁺ Ï€-complexes in the interstellar medium. Astronomy and Astrophysics, 2009, 494, 969-976.	5.1	29
48	Photodissociation of [Fex(C24H12)y]+ Complexes in the PIRENEA Setup: Iron-Polycyclic Aromatic Hydrocarbon Clusters as Candidates for Very Small Interstellar Grains. Journal of Physical Chemistry A, 2009, 113, 4878-4888.	2.5	29
49	Infrared Spectroscopy of [XFeC₂₄H₁₂]⁺ (X =) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 2 Phase: Experimental and Computational Studies of Astrophysical Interest. Journal of Physical Chemistry A, 2008, 112, 8551-8560.	2.5	37
50	Thermochemistry and Infrared Spectroscopy of Neutral and Cationic Ironâ"Polycyclic Aromatic Hydrocarbon Complexes of Astrophysical Interest:Â Fundamental Density Functional Theory Studies. Journal of Physical Chemistry A, 2007, 111, 9745-9755.	2.5	38
51	Fingerprint Vibrational Spectra of Protonated Methyl Esters of Amino Acids in the Gas Phase. Journal of the American Chemical Society, 2007, 129, 2829-2840.	13.7	81
52	Mid-IR spectroscopy of protonated leucine methyl ester performed with an FTICR or a Paul type ion-trap. International Journal of Mass Spectrometry, 2006, 249-250, 14-20.	1.5	123
53	Investigations of the clustering reactions of protonated amino acid esters by high pressure mass spectrometry and quantum chemical calculations. International Journal of Mass Spectrometry, 2006, 255-256, 301-311.	1.5	6
54	Infrared Multiphoton Dissociation Spectroscopy of Gas-Phase Mass-Selected Hydrocarbonâ"Fe+ Complexes. Journal of the American Chemical Society, 2004, 126, 11666-11674.	13.7	47

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55	Ultrasensitive spectroscopy of ionic reactive intermediates in the gas phase performed with the first coupling of an IR FEL with an FTICR-MS. Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2003, 507, 541-546.	1.6	84
56	Ultrasensitive spectroscopy of ionic reactive intermediates in the gas phase performed with the first coupling of an IR FEL with an FTICR-MS. , 2003, , 541-546.		2
57	Gas Phase Infrared Spectroscopy of Selectively Prepared Ions. Physical Review Letters, 2002, 89, 273002.	7.8	285
58	Towards the characterization of the mechanism of the sequential activation of four methane molecules by Ta+. International Journal of Mass Spectrometry, 2002, 219, 457-473.	1.5	20
59	Valence bond curve-crossing model of the 1,2-hydrogen shift in HCN and isovalent systems. Chemical Physics Letters, 2001, 350, 345-350.	2.6	7
60	Competition between agostic WCH2+ and HWCH+: A joint experimental and theoretical study. Journal of Chemical Physics, 2001, 115, 2510-2518.	3.0	22
61	Metal valence states inEu0.7NbO3,EuNbO3,andEu2Nb5O9by TB-LMTO-ASA band-structure calculations and resonant photoemission spectroscopy. Physical Review B, 1998, 57, 1510-1514.	3.2	15
62	Energetic processing of PAHs: isomerisation and dissociation. Chemical Modelling, 0, , 195-216.	0.4	3