Sylvain Picaud

List of Publications by Year
in descending order

133	3,075	126907	254184
papers	citations	33 h-index	43 g-index

133	133	133	2188
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Adsorption of organic compounds at the surface of Enceladusâ€™ ice grains. A grand canonical Monte Carlo simulation study. Molecular Simulation, 2022, 48, 19-30.	2.0	4
2	DFT Study of the Formation of Atmospheric Aerosol Precursors from the Interaction between Sulfuric Acid and Benzenedicarboxylic Acid Molecules. Journal of Physical Chemistry A, 2022, 126, 1211-1220.	2.5	2
3	Adsorption of C2â€“C5 alcohols on ice: A grand canonical Monte Carlo simulation study. Journal of Chemical Physics, 2022, 156, .	3.0	6
4	Formation of atmospheric molecular clusters from organic waste products and sulfuric acid molecules: a DFT study. Environmental Science Atmospheres, 2021, 1, 267-275.	2.4	2
5	Molecular Selectivity of CH₄â€“C₂H₆ Mixed Hydrates: A GCMC Study. ACS Earth and Space Chemistry, 2021, 5, 1782-1791.	2.7	3
6	Influence of Onion-like Carbonaceous Particles on the Aggregation Process of Hydrocarbons. ACS Omega, 2021, 6, 27898-27904.	3.5	2
7	Adsorption of CO and N2 molecules at the surface of solid water. A grand canonical Monte Carlo study. Journal of Chemical Physics, 2020, 153, 204502.	3.0	3
8	Molecular Selectivity of COâ€“N₂ Mixed Hydrates: Raman Spectroscopy and GCMC Studies. Journal of Physical Chemistry C, 2020, 124, 11886-11891.	3.1	7
9	Formation of Interstellar Complex Polycyclic Aromatic Hydrocarbons: Insights from Molecular Dynamics Simulations of Dehydrogenated Benzene. Astrophysical Journal, 2020, 900, 188.	4.5	16
10	Molecular-scale simulations of organic compounds on ice: application to atmospheric and interstellar sciences. Molecular Simulation, 2019, 45, 403-416.	2.0	8
11	Adsorption of Formamide at the Surface of Amorphous and Crystalline Ices under Interstellar and Tropospheric Conditions. A Grand Canonical Monte Carlo Simulation Study. Journal of Physical Chemistry A, 2019, 123, 2935-2948.	2.5	14
12	Hydrogen chloride adsorption on large defective PAHs modeling soot surfaces and influence on water trapping: A DFT and AIMD study. Chemical Physics, 2019, 523, 18-27.	1.9	9
13	Multiscale Modeling of Interfacial Oxidation Mechanism at Air/Organic Interface: Reactions of CH₂â•CH-Terminated Self-Assembled Monolayer with OH^{â€¢}, O₃, and HO₂^{â€¢}. Journal of Physical Chemistry C, 2018, 122, 9886-9898.	3.1	3
14	Ammonia Clathrate Hydrate As Seen from Grand Canonical Monte Carlo Simulations. ACS Earth and Space Chemistry, 2018, 2, 521-531.	2.7	20
15	Adsorption of Methylamine on Amorphous Ice under Interstellar Conditions. A Grand Canonical Monte Carlo Simulation Study. Journal of Physical Chemistry A, 2018, 122, 3398-3412.	2.5	14
16	Adsorption of Organic Molecules on Onion-like Carbons: Insights on the Formation of Interstellar Hydrocarbons. Astrophysical Journal, 2018, 867, 133.	4.5	21
17	A Grand Canonical Monte Carlo Study of the N₂, CO, and Mixed N₂â€“CO Clathrate Hydrates. Journal of Physical Chemistry C, 2018, 122, 18432-18444.	3.1	22
18	Analysis of Mixed Formic and Acetic Acid Aggregates Interacting With Water: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry C, 2017, 121, 13863-13875.	3.1	13

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19	Dependence of the adsorption of halogenated methane derivatives at the ice surface on their chemical structure. Journal of Molecular Liquids, 2017, 245, 17-26.	4.9	4
20	Adsorption of Chlorinated Methane Derivatives at the Ice Surface: A Grand Canonical Monte Carlo Simulation Study. Journal of Physical Chemistry C, 2017, 121, 7782-7793.	3.1	8
21	A DFT study of the interaction between large PAHs and atomic chlorine or hydrogen chloride molecule: Toward a modelling of the influence of chlorinated species on the trapping of water by soot. Chemical Physics, 2017, 483-484, 46-55.	1.9	3
22	Adsorption of Fluorinated Methane Derivatives at the Surface of Ice under Tropospheric Conditions, As Seen from Grand Canonical Monte Carlo Simulations. Journal of Physical Chemistry C, 2016, 120, 17386-17399.	3.1	19
23	Adsorption of Methylamine at the Surface of Ice. A Grand Canonical Monte Carlo Simulation Study. Journal of Physical Chemistry C, 2016, 120, 23480-23489.	3.1	12
24	Martian zeolites as a source of atmospheric methane. Icarus, 2016, 278, 1-6.	2.5	16
25	A â^¼32â€“70 K FORMATION TEMPERATURE RANGE FOR THE ICE GRAINS AGGLOMERATED BY COMET 67 P/CHURYUMOVâ€“GERASIMENKO. Astrophysical Journal Letters, 2015, 805, L1.	8.3	22
26	Methane Clathrates in the Solar System. Astrobiology, 2015, 15, 308-326.	3.0	62
27	Molecular Dynamics Simulations of the Interaction between Water Molecules and Aggregates of Acetic or Propionic Acid Molecules. Journal of Physical Chemistry B, 2015, 119, 15662-15674.	2.6	24
28	The effect of anaesthetics on the properties of a lipid membrane in the biologically relevant phase: a computer simulation study. Physical Chemistry Chemical Physics, 2015, 17, 14750-14760.	2.8	31
29	Possible evidence for a methane source in Enceladus' ocean. Geophysical Research Letters, 2015, 42, 1334-1339.	4.0	65
30	Calculations of the mass absorption cross sections for carbonaceous nanoparticles modeling soot. Journal of Quantitative Spectroscopy and Radiative Transfer, 2015, 164, 69-81.	2.3	19
31	A simple vanâ€™t Hoff law for calculating Langmuir constants in clathrate hydrates. Chemical Physics, 2015, 448, 53-60.	1.9	12
32	Adsorption of Methylene Fluoride and Methylene Chloride at the Surface of Ice under Tropospheric Conditions: A Grand Canonical Monte Carlo Simulation Study. Journal of Physical Chemistry C, 2015, 119, 17243-17252.	3.1	14
33	Water and formic acid aggregates: A molecular dynamics study. Journal of Chemical Physics, 2014, 141, 104701.	3.0	17
34	Adsorption of H2O2 at the surface of Ih ice, as seen from grand canonical Monte Carlo simulations. Chemical Physics Letters, 2014, 600, 73-78.	2.6	12
35	First-Principles Study of the Interaction between NO and Large Carbonaceous Clusters Modeling the Soot Surface. Journal of Physical Chemistry A, 2014, 118, 1443-1450.	2.5	21
36	On the Abundances of Noble and Biologically Relevant Gases in Lake Vostok, Antarctica. Astrobiology, 2013, 13, 380-390.	3.0	14

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37	Adsorption of atmospheric oxidants at divacancy sites of graphene: A DFT study. Computational and Theoretical Chemistry, 2013, 1016, 22-27.	2.5	23
38	Adsorption of Aromatic Hydrocarbon Molecules at the Surface of Ice, As Seen by Grand Canonical Monte Carlo Simulation. Journal of Physical Chemistry C, 2013, 117, 6719-6729.	3.1	38
39	Molecular dynamics simulations of the water adsorption around malonic acid aerosol models. Physical Chemistry Chemical Physics, 2013, 15, 10942.	2.8	17
40	Volatile Trapping in Martian Clathrates. Space Science Reviews, 2013, 174, 213-250.	8.1	39
41	Anesthetic molecules embedded in a lipid membrane: a computer simulation study. Physical Chemistry Chemical Physics, 2012, 14, 12956.	2.8	27
42	Adsorption of Acetaldehyde on Ice As Seen from Computer Simulation and Infrared Spectroscopy Measurements. Langmuir, 2012, 28, 4198-4207.	3.5	25
43	Structure and reactivity of carbon multivacancies in graphene. Computational and Theoretical Chemistry, 2012, 990, 159-166.	2.5	18
44	Mars cryosphere: A potential reservoir for heavy noble gases?. Icarus, 2012, 218, 80-87.	2.5	14
45	The Iceâ^'Vapor Interface and the Melting Point of Ice I_h for the Polarizable POL3 Water Model. Journal of Physical Chemistry A, 2011, 115, 5973-5982.	2.5	19
46	Water adsorption around oxalic acid aggregates: a molecular dynamics simulation of water nucleation on organic aerosols. Physical Chemistry Chemical Physics, 2011, 13, 19830.	2.8	24
47	ON THE VOLATILE ENRICHMENTS AND HEAVY ELEMENT CONTENT IN HD189733b. Astrophysical Journal, 2011, 727, 77.	4.5	38
48	REMOVAL OF TITAN'S ATMOSPHERIC NOBLE GASES BY THEIR SEQUESTRATION IN SURFACE CLATHRATES. Astrophysical Journal Letters, 2011, 740, L9.	8.3	28
49	A new semi-empirical model for the oxidation of polycyclic aromatic hydrocarbon (PAHs) molecules physisorbed on soot. II. Application to the reaction PAH+OH for a series of large PAH molecules. Computational and Theoretical Chemistry, 2011, 965, 259-267.	2.5	3
50	IMPACT REGIMES AND POST-FORMATION SEQUESTRATION PROCESSES: IMPLICATIONS FOR THE ORIGIN OF HEAVY NOBLE GASES IN TERRESTRIAL PLANETS. Astrophysical Journal, 2010, 714, 1418-1423.	4.5	9
51	Water Adsorption on Oxidized Single Atomic Vacancies Present at the Surface of Small Carbonaceous Nanoparticles Modeling Soot. ChemPhysChem, 2010, 11, 4088-4096.	2.1	15
52	Molecular Dynamics Simulation of the Adsorption of Oxalic Acid on an Ice Surface. ChemPhysChem, 2010, 11, 3971-3979.	2.1	14
53	Adsorption of Hydroxyacetone on Pure Ice Surfaces. ChemPhysChem, 2010, 11, 3921-3927.	2.1	11
54	Interaction of water molecules with defective carbonaceous clusters: An ab initio study. Surface Science, 2010, 604, 1666-1673.	1.9	34

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55	A theoretical characterization of the interaction of water with oxidized carbonaceous clusters. Carbon, 2010, 48, 1570-1579.	10.3	26
56	Sensitivity of predicted gas hydrate occupancies on treatment of intermolecular interactions. Journal of Chemical Physics, 2010, 132, 104510.	3.0	8
57	Water adsorption isotherms on porous onionlike carbonaceous particles. Simulations with the grand canonical Monte Carlo method. Journal of Chemical Physics, 2010, 133, 144702.	3.0	36
58	Adsorption of Benzaldehyde at the Surface of Ice, Studied by Experimental Method and Computer Simulation. Langmuir, 2010, 26, 9596-9606.	3.5	29
59	Volatile inventories in clathrate hydrates formed in the primordial nebula. Faraday Discussions, 2010, 147, 509.	3.2	62
60	CLATHRATION OF VOLATILES IN THE SOLAR NEBULA AND IMPLICATIONS FOR THE ORIGIN OF TITAN'S ATMOSPHERE. Astrophysical Journal, 2009, 691, 1780-1786.	4.5	70
61	Pressure reversal of general anaesthetics: A possible mechanism from molecular dynamics simulations. Journal of Molecular Liquids, 2009, 147, 128-134.	4.9	14
62	Incorporation of argon, krypton and xenon into clathrates on Mars. Icarus, 2009, 203, 66-70.	2.5	20
63	Bottom-up multi-step approach to study the relations between the structure and the optical properties of carbon soot nanoparticles. Journal of Quantitative Spectroscopy and Radiative Transfer, 2009, 110, 1615-1627.	2.3	6
64	Variability of the methane trapping in martian subsurface clathrate hydrates. Planetary and Space Science, 2009, 57, 42-47.	1.7	42
65	A new semi-empirical model for the oxidation of PAHs physisorbed on soot. I. Application to the reaction C₆H₆+OH. Molecular Simulation, 2009, 35, 1130-1139.	2.0	2
66	Optical properties of soot nanoparticles. Journal of Quantitative Spectroscopy and Radiative Transfer, 2008, 109, 1791-1801.	2.3	20
67	A theoretical investigation into the trapping of noble gases by clathrates on Titan. Planetary and Space Science, 2008, 56, 1607-1617.	1.7	36
68	Adsorption of water molecules on partially oxidized graphite surfaces: a molecular dynamics study of the competition between OH and COOH sites,. Physical Chemistry Chemical Physics, 2008, 10, 6998.	2.8	35
69	Investigation of the adsorption behaviour of acetone at the surface of ice. A grand canonical Monte Carlo simulation study. Physical Chemistry Chemical Physics, 2008, 10, 6369.	2.8	41
70	Adsorption Isotherm of Formic Acid on the Surface of Ice, as Seen from Experiments and Grand Canonical Monte Carlo Simulation. Journal of Physical Chemistry C, 2008, 112, 8976-8987.	3.1	51
71	Molecular Dynamics and Monte Carlo Simulations of Organic Compounds Adsorbed on Ice Surfaces. AIP Conference Proceedings, 2007, , .	0.4	2
72	Grand canonical Monte Carlo simulation of the adsorption isotherms of water molecules on model soot particles. Journal of Chemical Physics, 2007, 127, 164719.	3.0	36

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73	Adsorption of Phenanthrene on Natural Snow. Environmental Science & Technology, 2007, 41, 6033-6038.	10.0	48
74	Free-Energy Profile of Small Solute Molecules at the Free Surfaces of Water and Ice, as Determined by Cavity Insertion Widom Calculations. Journal of Physical Chemistry C, 2007, 111, 9407-9416.	3.1	45
75	Calculation of the Adsorption Isotherm of Formaldehyde on Ice by Grand Canonical Monte Carlo Simulation. Journal of Physical Chemistry C, 2007, 111, 14170-14178.	3.1	37
76	Clathrate hydrates as a sink of noble gases in Titan's atmosphere. Astronomy and Astrophysics, 2007, 474, L17-L20.	5.1	44
77	A possible mechanism for pressure reversal of general anaesthetics from molecular simulations. Chemical Physics Letters, 2007, 438, 294-297.	2.6	17
78	Photodissociation of a HCl molecule adsorbed on ice at T=210K. Surface Science, 2007, 601, 3034-3041.	1.9	8
79	Molecular Dynamics Simulation Study of Water Adsorption on Hydroxylated Graphite Surfaces. Journal of Physical Chemistry B, 2006, 110, 8398-8408.	2.6	30
80	Molecular dynamics study of diffusion of formaldehyde in ice. Chemical Physics Letters, 2006, 432, 78-83.	2.6	20
81	A semi-empirical potential model for calculating interactions between large aromatic molecules and graphite surfaces. Computational and Theoretical Chemistry, 2006, 772, 1-12.	1.5	16
82	Dynamics of TIP5P and TIP4P/ice potentials. Journal of Chemical Physics, 2006, 125, 174712.	3.0	24
83	A grand canonical Monte-Carlo simulation study of water adsorption on a model soot particle. Molecular Simulation, 2006, 32, 487-493.	2.0	25
84	Determination of the Adsorption Isotherm of Methanol on the Surface of Ice. An Experimental and Grand Canonical Monte Carlo Simulation Study. Journal of the American Chemical Society, 2006, 128, 15300-15309.	13.7	72
85	Ab initio study of the water adsorption on hydroxylated graphite surfaces. Chemical Physics Letters, 2005, 406, 430-435.	2.6	49
86	Molecular dynamics simulations of polarizable nanotubes interacting with water. Physical Review B, 2005, 71, .	3.2	52
87	Adsorption of acetic acid on ice: Experiments and molecular dynamics simulations. Journal of Chemical Physics, 2005, 122, 194707.	3.0	46
88	Clustering of water molecules on model soot particles: an ab initio study. Computing Letters, 2005, 1, 277-287.	0.5	26
89	A molecular dynamics simulation of the electrical conductivity behaviors of highly concentrated liquid ammoniates Nalâ^™Î±NH3: Comparison with experimental measurements. Journal of Chemical Physics, 2005, 122, 171102.	3.0	2
90	Structure of the neopentane monolayer adsorbed on MgO(001): experiments and calculations. Surface Science, 2004, 550, 133-139.	1.9	3

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91	Comparison between methanol and formaldehyde adsorption on ice: a molecular dynamics study. Chemical Physics Letters, 2004, 393, 457-463.	2.6	36
92	Molecular dynamics simulations of chloroform on ice. Physical Chemistry Chemical Physics, 2004, 6, 1970-1974.	2.8	7
93	Theoretical Study of the Adsorption of Water on a Model Soot Surface:Â I. Quantum Chemical Calculations. Journal of Physical Chemistry B, 2004, 108, 5405-5409.	2.6	43
94	Theoretical Study of the Adsorption of Water on a Model Soot Surface:Â II. Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2004, 108, 5410-5415.	2.6	44
95	Experimental and Theoretical Adsorption Study of Ethanol on Ice Surfaces. Journal of Physical Chemistry B, 2004, 108, 17425-17432.	2.6	37
96	Combined elastic neutron scattering experiments and molecular dynamics simulations on the concentrated liquid electrolyte NaIÂ·3.3NH3. Journal of Molecular Liquids, 2003, 108, 1-19.	4.9	4
97	The effect of HCl adsorption on the structure and dynamics of the ice surface. Canadian Journal of Physics, 2003, 81, 415-422.	1.1	2
98	Adsorption of HF and HCl molecules on ice at 190 and 235 K from molecular dynamics simulations: Free energy profiles and residence times. Journal of Chemical Physics, 2003, 118, 9814-9823.	3.0	24
99	Structure and dynamics of ice Ih films upon HCl adsorption between 190 and 270 K. II. Molecular dynamics simulations. Journal of Chemical Physics, 2002, 116, 5150.	3.0	24
100	Structure and dynamics of ice Ih films upon HCl adsorption between 190 and 270 K. I. Neutron diffraction and quasielastic neutron scattering experiments. Journal of Chemical Physics, 2002, 116, 5143.	3.0	21
101	Geometry and dynamics of formic and acetic acids adsorbed on ice. Chemical Physics Letters, 2002, 365, 1-7.	2.6	48
102	The structure of the c(4Ã—2) CO/MgO() monolayer revisited by neutron diffraction. Surface Science, 2001, 494, 206-212.	1.9	6
103	Dynamics of ice layers deposited on MgO(001): Quasielastic neutron scattering experiments and molecular dynamics simulations. Journal of Chemical Physics, 2001, 114, 6371-6381.	3.0	26
104	Time study of pollutants at the surface of ice at 200 K. Chemical Physics Letters, 2000, 329, 331-335.	2.6	12
105	Adsorption of acetone molecules on proton ordered ice. A molecular dynamics study. Journal of Chemical Physics, 2000, 112, 9898-9908.	3.0	54
106	Experimental and theoretical studies of acetylene layers adsorbed on KCl(001). Physical Review B, 2000, 61, 14028-14036.	3.2	12
107	Monolayers of acetone and methanol molecules on ice. Surface Science, 2000, 454-456, 178-182.	1.9	26
108	The passage of small molecules through a water film supported by MgO(100): Transfer times from molecular dynamics simulations. Journal of Chemical Physics, 2000, 113, 1184-1193.	3.0	7

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109	Monolayers of ortho-H2, para-H2, para-D2 and normal-H2 adsorbed on NaCl(001) single crystal surfaces. Journal of Chemical Physics, 1999, 110, 2566-2578.	3.0	22
110	Quantum description of the hindered rotor motion ofCH4adsorbed on MgO(100) and He-bound state analysis. Physical Review B, 1999, 60, 8333-8342.	3.2	12
111	Adsorption of small polar molecules as a probe of the surface electric field created by water layers supported by MgO(100): a theoretical study. Chemical Physics, 1999, 244, 227-249.	1.9	13
112	Water monolayers on MgO(100): structural investigations by LEED experiments, tensor LEED dynamical analysis and potential calculations. Surface Science, 1998, 409, 101-116.	1.9	88
113	Adsorption of ortho and para H2 on NaCl(001). Journal of Chemical Physics, 1998, 109, 6435-6449.	3.0	25
114	Adsorption of water on MgO(100): A singular behavior. Physical Review B, 1998, 57, 11931-11934.	3.2	26
115	A molecular dynamics study of the structure of water layers adsorbed on MgO(100). Journal of Chemical Physics, 1998, 109, 3245-3254.	3.0	59
116	Phonon-libron dynamics of acetylene adsorbed onNaCl(001). Physical Review B, 1998, 57, 10090-10099.	3.2	13
117	Experimental and theoretical studies of the monolayer structure of OCS adsorbed on NaCl(001): Coexistence of orientationally inequivalent phases. Journal of Chemical Physics, 1997, 106, 5271-5283.	3.0	12
118	He-diffraction investigation of the (1 Ã— 1) CO phase on NaCl(100): a fully quantum study. Surface Science, 1996, 347, 128-142.	1.9	9
119	On the difficulty for finding the orientational geometries of adsorbed monolayers: illustration with the system. Surface Science, 1996, 360, 261-270.	1.9	20
120	Structure of CO monolayer adsorbed on NaCl(100) from molecular dynamics. Journal of Chemical Physics, 1996, 105, 8453-8462.	3.0	26
121	Dynamical model for the interpretation of the geometry of the (4Ã—2) CO layer adsorbed on MgO (001). Physical Review B, 1996, 53, 16615-16620.	3.2	13
122	Molecule-step interactions in the aggregation of admolecules on ionic substrates. Chemical Physics Letters, 1995, 242, 212-220.	2.6	6
123	Molecular adsorption on ionic substrates: Characterization of terrace and step sites. Chemical Physics, 1995, 194, 65-80.	1.9	24
124	Vibrational infrared spectrum of NH3 adsorbed on MgO(100). II. Interatomic potential calculations. Chemical Physics, 1995, 201, 73-85.	1.9	12
125	Phonon-libron dynamics of a commensurate molecular monolayer: (2Ã—1)CO2/NaCl(100). Physical Review B, 1995, 52, 2144-2153.	3.2	7
126	Interpretation of the polarization infrared spectrum of CO2 monolayers adsorbed on ionic substrates. Journal of Chemical Physics, 1995, 102, 7229-7237.	3.0	17

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127	A Comparitive Study of the Geometry of CO ₂ Monolayers Adsorbed on the Ionic Substrates NaCl and MgO(100). Europhysics Letters, 1994, 25, 131-136.	2.0	27
128	Adsorption of polar molecules on substrates with strong electric surface fields: from aggregates to monolayers. Chemical Physics Letters, 1993, 209, 340-346.	2.6	45
129	Theoretical study of the monolayer structures of CO adsorbed on NaCl(100). Surface Science, 1993, 294, 149-160.	1.9	48
130	NH3 physisorption on MgO(100) substrate. Potential calculations revisited. Journal of Chemical Physics, 1993, 98, 3488-3495.	3.0	30
131	Geometry of (NH3)n and (H2O)n aggregates adsorbed on well characterized MgO(100) and Si(111)-(1 Ã—) Tj ETQq1 1 0.784314 rgB	1.9	35
132	Ammonia and water physisorption on a H-passivated Si(111) surface: a study of admolecule motions. Surface Science, 1992, 272, 172-181.	1.9	2
133	Molecular physisorption on atom-adsorbed unreconstructed (111) silicon surfaces. Surface Science, 1991, 258, 210-224.	1.9	11