

Alfredo Juan

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

84
papers

1,120
citations

19
h-index

29
g-index

86
ext. papers

1,258
ext. citations

4.6
avg, IF

4.48
L-index

#	Paper	IF	Citations
84	Theoretical study of the octahedral substitution effect in delaminated pyrophyllite: physicochemical properties and applications. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 14601-14607 ^{3.6}		
83	Experimental and DFT Studies of Hybrid Silver/Cdots Nanoparticles. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 2425-2435	3.4	3
82	Molecular dynamics simulations on interaction of ssDNA-causing DM1 with carbon and boron nitride nanotubes to inhibit the formation of CTG repeat secondary structures. <i>Applied Surface Science</i> , 2020 , 524, 146572	6.7	7
81	Ultra-low concentration protein detection based on phenylalanine-Pd/SWCNT as a high sensitivity nanoreceptor.. <i>RSC Advances</i> , 2020 , 10, 2650-2660	3.7	10
80	Influence of functionalization, surface area and charge distribution of SBA15-based adsorbents on CO (II) and NI (II) removal from aqueous solutions. <i>Journal of Environmental Chemical Engineering</i> , 2020 , 8, 103671	6.8	4
79	DFT study of ethanol adsorption on CaO(0 0 1) surface. <i>Applied Surface Science</i> , 2020 , 500, 144254	6.7	6
78	Adsorption of bentazone and imazapyr from water by using functionalized silica: Experimental and computational analysis. <i>Journal of Contaminant Hydrology</i> , 2019 , 227, 103542	3.9	8
77	Detection of oxytetracycline in honey using SERS on silver nanoparticles. <i>TrAC - Trends in Analytical Chemistry</i> , 2019 , 121, 115673	14.6	12
76	Zero energy mode for an electron in graphene in a perpendicular magnetic field with constant asymptotics. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2019 , 109, 225-227	3	1
75	Theoretical study of the role of the interface of Ag4 nanoclusters deposited on TiO ₂ (110) and TiO ₂ (101). <i>Applied Surface Science</i> , 2019 , 490, 343-351	6.7	12
74	Ruthenium decorated single walled carbon nanotube for molecular hydrogen storage: A first-principle study. <i>International Journal of Hydrogen Energy</i> , 2019 , 44, 8376-8383	6.7	21
73	Adsorption of bentazon on CAT and CARBOPAL activated carbon: Experimental and computational study. <i>Applied Surface Science</i> , 2018 , 433, 487-501	6.7	8
72	Hydrogen storage in Zr _{0.9} Ti _{0.1} (Ni _{0.5} Cr _{0.5-x} V _x) ₂ Laves phase, with x=0, 0.125, 0.25, 0.375, 0.5. A theoretical approach. <i>International Journal of Hydrogen Energy</i> , 2018 , 43, 16085-16091	6.7	4
71	Adsorption and removal of phenoxy acetic herbicides from water by using commercial activated carbons: experimental and computational studies. <i>Journal of Contaminant Hydrology</i> , 2018 , 218, 84-93	3.9	26
70	Surface enhancement Raman spectroscopy and density functional theory study of silver nanoparticles synthesized with d-glucose. <i>Journal of Raman Spectroscopy</i> , 2018 , 49, 1756-1764	2.3	10
69	Analytic solution for gauged Dirac-Weyl equation in (2 + 1)-dimensions. <i>Europhysics Letters</i> , 2017 , 118, 21001	1.6	1
68	Redox behavior of a low-doped Pr-CeO ₂ (111) surface. A DFT+U study. <i>Applied Surface Science</i> , 2017 , 401, 206-217	6.7	15

67	Rhodium clustering process on defective (8,0) SWCNT: Analysis of chemical and physical properties using density functional theory. <i>Applied Surface Science</i> , 2017 , 425, 823-832	6.7	10
66	DFT study of D-glucose adsorption on single-walled carbon nanotubes decorated with platinum. A bonding analysis. <i>Applied Surface Science</i> , 2017 , 423, 542-548	6.7	4
65	Synthesis and Characterization of Silver Nanoparticles Prepared with Honey: The Role of Carbohydrates. <i>Analytical Letters</i> , 2017 , 50, 877-888	2.2	19
64	DFT study of Rh-decorated pristine, B-doped and vacancy defected graphene for hydrogen adsorption. <i>RSC Advances</i> , 2016 , 6, 83926-83941	3.7	27
63	A DFT study of hydrogen storage in Zr(Cr 0.5 Ni 0.5) 2 Laves phase. <i>International Journal of Hydrogen Energy</i> , 2016 , 41, 2700-2710	6.7	11
62	A van der Waals DFT study of PtH ₂ systems adsorbed on pristine and defective graphene. <i>Applied Surface Science</i> , 2016 , 382, 80-87	6.7	18
61	Geometrical and Electronic Properties of Hydrated Sodium Montmorillonite and Tetracycline Montmorillonite from DFT Calculations. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 16082-16088	3.8	15
60	A DFT study of phenol adsorption on a low doping MnTe composite oxide model. <i>Applied Surface Science</i> , 2015 , 359, 14-20	6.7	13
59	Valley properties of doped graphene in a magnetic field. <i>European Physical Journal B</i> , 2015 , 88, 1	1.2	10
58	Propylene Adsorption On a Nonstoichiometric VSbO ₄ (110) Surface. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 4967-4975	3.8	2
57	A Theoretical Study of the Effect of Zr-, Nb-Doped and Vacancy-like Defects on H Desorption on MgH ₂ (110) Surface. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 4231-4237	3.8	17
56	Ultrathin (0 0 1) and (1 0 0) TiO ₂ (B) sheets: Surface reactivity and structural properties. <i>Applied Surface Science</i> , 2014 , 290, 180-187	6.7	24
55	Selenium adsorption at different coverages on Fe(1 0 0) and Fe(1 1 1): A DFT study. <i>Applied Surface Science</i> , 2014 , 315, 252-260	6.7	10
54	Theoretical Study of Hydrogen Adsorption on Ru-Decorated (8,0) Single-Walled Carbon Nanotube. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 27672-27680	3.8	36
53	Density functional theory study of water interactions on Mn-doped CeO ₂ (1 1 1) surface. <i>Applied Surface Science</i> , 2014 , 313, 784-793	6.7	13
52	A DFT study of cyclopropane adsorption on Pt(1 1 1). Electronic structure and bonding. <i>Applied Surface Science</i> , 2014 , 303, 324-330	6.7	1
51	Bonding in PdH ₂ and Pd ₂ H ₂ systems adsorbed on carbon nanotubes: Implications for hydrogen storage. <i>International Journal of Hydrogen Energy</i> , 2014 , 39, 8780-8790	6.7	21
50	A DFT study of dopant (Zr, Nb) and vacancies on the dehydrogenation on MgH ₂ (001) surface. <i>International Journal of Hydrogen Energy</i> , 2014 , 39, 1732-1739	6.7	11

49	Mn-Doped CeO ₂ : DFT+U Study of a Catalyst for Oxidation Reactions. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 18063-18073	3.8	53
48	The Effect of Metal Vacancies on Vanadium Antimonate Surface Properties. A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2013 , 117, 20548-20556	3.8	3
47	THE OBSERVABLE-STATE MODEL AND NONRENORMALIZABLE THEORIES. <i>International Journal of Modern Physics A</i> , 2013 , 28, 1350016	1.2	2
46	Benzene adsorption on PtCo(1 1 1): A DFT study. <i>Applied Surface Science</i> , 2013 , 282, 17-24	6.7	7
45	The adsorption of acrolein on a Pt (111): A study of chemical bonding and electronic structure. <i>Applied Surface Science</i> , 2012 , 263, 79-85	6.7	9
44	Theoretical Model for CO Adsorption and Dissociation on Clean and K-Doped Mo ₂ C Surfaces. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 24573-24581	3.8	25
43	Adsorption of ammonia on vanadium-antimony mixed oxides. <i>Applied Surface Science</i> , 2012 , 258, 3617-3623	6.7	9
42	DFT study of H ₂ adsorption on Pd-decorated single walled carbon nanotubes with C-vacancies. <i>International Journal of Hydrogen Energy</i> , 2012 , 37, 10156-10164	6.7	30
41	Oxygen vacancy formation on the Ni/Ce _{0.75} Zr _{0.25} O ₂ (111) surface. A DFT+U study. <i>International Journal of Hydrogen Energy</i> , 2012 , 37, 14937-14944	6.7	12
40	The adsorption of CO on potassium doped molybdenum carbide surface: An ab-initio study. <i>Catalysis Today</i> , 2012 , 181, 102-107	5.3	12
39	DFT Study of Hydrogen Adsorption on Palladium Decorated Graphene. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 4315-4323	3.8	117
38	Advanced materials for hydrogen storage based on iron-palladium intermetallic alloys. <i>Inorganic Materials: Applied Research</i> , 2011 , 2, 172-175	0.6	0
37	A First-Principles Modeling of Ni Interactions on CeO ₂ /ZrO ₂ Mixed Oxide Solid Solutions. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 7456-7465	3.8	26
36	Density functional theory study of selenium adsorption on Fe(1 1 0). <i>Applied Surface Science</i> , 2011 , 257, 6878-6883	6.7	5
35	The influence of Mg on the C adsorption on Ni(1 0 0): A DFT study. <i>Journal of Molecular Catalysis A</i> , 2010 , 315, 171-177		7
34	A bonding study of CO/benzene co-adsorption on Rh(111). <i>Journal of Molecular Catalysis A</i> , 2010 , 323, 23-27		3
33	Effects of potassium on the adsorption of methanol on Mo ₂ C(001) surface. <i>Surface Science</i> , 2010 , 604, 914-919	1.8	24
32	Hydrogen and carbon interaction in a FeNi alloy with a vacancy. <i>Physica Status Solidi (B): Basic Research</i> , 2009 , 246, 1275-1285	1.3	3

31	The hydrogen effect in the electronic structure and bonding of the B2 FeAl alloy with a Fe vacancy. <i>International Journal of Hydrogen Energy</i> , 2009 , 34, 9591-9595	6.7	6
30	A theoretical study of cyclopentene (c-C ₅ H ₈) dehydrogenation to cyclopentadienyl anion (c-C ₅ H ₅ ⁻) on Ni (111). <i>Journal of Molecular Catalysis A</i> , 2009 , 314, 28-34		7
29	THE CO-ADSORPTION OF BENZENE AND CO ON Co(0001). <i>Surface Review and Letters</i> , 2009 , 16, 749-755	1.1	5
28	Theoretical study of the influence of cation vacancies on the catalytic properties of vanadium antimonate. <i>Applied Surface Science</i> , 2008 , 254, 5837-5843	6.7	4
27	The effect of carbon on the electronic structure of FeNi alloys with a stacking fault. <i>Physica Status Solidi (B): Basic Research</i> , 2008 , 245, 2771-2778	1.3	0
26	A DFT study of H adsorption on Pt(111) and PtRu(111) surfaces. <i>Applied Surface Science</i> , 2008 , 254, 5827-5830	6.7	7
25	ADSORPTION OF HYDROGEN ON Ga ₂ O ₃ (100): A THEORETICAL STUDY. <i>Surface Review and Letters</i> , 2007 , 14, 79-86	1.1	6
24	A theoretical study of the electronic structure and bonding of the monoclinic phase of Mg ₂ NiH ₄ . <i>International Journal of Hydrogen Energy</i> , 2007 , 32, 4943-4948	6.7	29
23	The effect of interstitial hydrogen on the electronic structure of the B2 FeAl alloy. <i>Physica Status Solidi (B): Basic Research</i> , 2007 , 244, 3684-3694	1.3	6
22	Benzene and NO on a Ru(001) surface: Electronic structure and bonding. <i>Applied Surface Science</i> , 2006 , 252, 2108-2114	6.7	3
21	Theoretical study of hydrogen adsorption on FePd face-centered cubic alloy surfaces. <i>Physical Review B</i> , 2005 , 71,	3.3	20
20	The electronic structure of vanadium antimonate. <i>Catalysis Today</i> , 2005 , 107-108, 40-45	5.3	5
19	Hydrogen adsorption on Ga ₂ O ₃ (1 0 0) surface containing oxygen vacancies. <i>Surface Science</i> , 2005 , 575, 171-180	1.8	40
18	Density functional study of H-Fe vacancy interaction in bcc iron. <i>Journal of Physics Condensed Matter</i> , 2004 , 16, 6907-6916	1.8	8
17	The adsorption of hydrogen on face centered tetragonal FePd surfaces. <i>Solid State Communications</i> , 2004 , 131, 81-85	1.6	9
16	The effect of interstitial hydrogen on the electronic structure of FePd alloys. <i>Journal of Physics and Chemistry of Solids</i> , 2004 , 65, 1799-1807	3.9	18
15	Benzene and carbon monoxide co-adsorption on Pt(1 1 1): a theoretical study. <i>Applied Surface Science</i> , 2004 , 236, 394-405	6.7	13
14	THE EFFECT OF H ON THE ELECTRONIC STRUCTURE OF AN Fe(110)Pd(100) INTERFACE. <i>Surface Review and Letters</i> , 2003 , 10, 879-888	1.1	3

13	The Electronic Structure and Bonding of MAO on the SiO ₂ (111) Hydrated Surface. <i>Macromolecular Theory and Simulations</i> , 2001 , 10, 485-490	1.5	2
12	Zirconocene interaction with MAO on (111) and (100) silica surfaces. <i>Macromolecular Theory and Simulations</i> , 2000 , 9, 381-387	1.5	2
11	A theoretic study of the indene adsorption on SiO ₂ surfaces. <i>Computational Materials Science</i> , 2000 , 17, 61-72	3.2	2
10	CO on Pd(100)/SiO ₂ : a computational study of the effect of CaO on the energetics of adsorption. <i>Computational Materials Science</i> , 2000 , 18, 39-47	3.2	1
9	Hydrogen on the Fe(110) surface and near bulk bcc Fe vacancies. <i>Surface Science</i> , 1999 , 421, 1-16	1.8	72
8	A computational simulation for H-dislocated BCC Fe interaction. <i>Materials Chemistry and Physics</i> , 1998 , 55, 61-67	4.4	4
7	Preparation and characterization of Al ₂ O ₃ -supported Pd Mo catalysts. <i>Applied Catalysis B: Environmental</i> , 1998 , 15, 115-127	21.8	25
6	A computer-aided modelling analogue for lattice dynamics. <i>European Journal of Physics</i> , 1997 , 18, 398-403		1
5	Adsorption/Oxidation of CH ₃ OH on V ₂ O ₅ . A Theoretical and Experimental Study. <i>Adsorption Science and Technology</i> , 1997 , 15, 517-529	3.6	3
4	Catalytic oxidation of CH ₃ OH to HCOOCH ₃ on V ₂ O ₅ : A theoretical study. <i>Journal of Molecular Catalysis A</i> , 1997 , 118, 283-291		28
3	The Co-adsorption of tetramethylpiperidine and TiCl ₄ on MgCl ₂ . A theoretical study of a Ziegler-Natta pre-catalyst. <i>Journal of Molecular Catalysis A</i> , 1997 , 122, 25-37		22
2	Characterization of RuMoBiO ₂ catalysts. A comparative study before and after CO hydrogenation reaction. <i>Journal of Materials Chemistry</i> , 1996 , 6, 1433-1439		3
1	Planck's constant determination using a light bulb. <i>American Journal of Physics</i> , 1996 , 64, 819-821	0.7	9