Alfredo Juan

List of Publications by Citations

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	DFT Study of Hydrogen Adsorption on Palladium Decorated Graphene. *Journal of Physical Chemistry C*, **2011**, 115, 4315-4323	3.8	117
83	Hydrogen on the Fe(110) surface and near bulk bcc Fe vacancies. *Surface Science*, **1999**, 421, 1-16	1.8	72
82	Mn-Doped CeO2: DFT+U Study of a Catalyst for Oxidation Reactions. *Journal of Physical Chemistry C* , **2013**, 117, 18063-18073	3.8	53
81	Hydrogen adsorption on Ga2O3(1 0 0) surface containing oxygen vacancies. *Surface Science*, **2005** , 575, 171-180	1.8	40
80	Theoretical Study of Hydrogen Adsorption on Ru-Decorated (8,0) Single-Walled Carbon Nanotube. *Journal of Physical Chemistry C*, **2014**, 118, 27672-27680	3.8	36
79	DFT study of H2 adsorption on Pd-decorated single walled carbon nanotubes with C-vacancies. *International Journal of Hydrogen Energy*, **2012**, 37, 10156-10164	6.7	30
78	A theoretical study of the electronic structure and bonding of the monoclinic phase of Mg2NiH4Mg2NiH4. *International Journal of Hydrogen Energy*, **2007**, 32, 4943-4948	6.7	29
77	Catalytic oxidation of CH3OH to HCOOCH3 on V2O5: A theoretical study. *Journal of Molecular Catalysis A*, **1997**, 118, 283-291		28
76	DFT study of Rh-decorated pristine, B-doped and vacancy defected graphene for hydrogen adsorption. *RSC Advances*, **2016**, 6, 83926-83941	3.7	27
75	A First-Principles Modeling of Ni Interactions on CeO2ZrO2 Mixed Oxide Solid Solutions. *Journal of Physical Chemistry C*, **2011**, 115, 7456-7465	3.8	26
74	Adsorption and removal of phenoxy acetic herbicides from water by using commercial activated carbons: experimental and computational studies. *Journal of Contaminant Hydrology*, **2018**, 218, 84-93	3.9	26
73	Theoretical Model for CO Adsorption and Dissociation on Clean and K-Doped Mo2C Surfaces. *Journal of Physical Chemistry C*, **2012**, 116, 24573-24581	3.8	25
72	Preparation and characterization of Al2O3-supported Pd Mo catalysts. *Applied Catalysis B: Environmental*, **1998**, 15, 115-127	21.8	25
71	Ultrathin (0 0 1) and (1 0 0) TiO2(B) sheets: Surface reactivity and structural properties. *Applied Surface Science*, **2014**, 290, 180-187	6.7	24
70	Effects of potassium on the adsorption of methanol on Mo2C(001) surface. *Surface Science*, **2010**, 604, 914-919	1.8	24
69	The Co-adsorption of tetramethylpiperidine and TiCl4 on MgCl2. A theoretical study of a Ziegler-Natta pre-catalyst. *Journal of Molecular Catalysis A*, **1997**, 122, 25-37		22
68	Bonding in PdH2 and Pd2H2 systems adsorbed on carbon nanotubes: Implications for hydrogen storage. *International Journal of Hydrogen Energy*, **2014**, 39, 8780-8790	6.7	21

67	Ruthenium decorated single walled carbon nanotube for molecular hydrogen storage: A first-principle study. *International Journal of Hydrogen Energy*, **2019**, 44, 8376-8383	6.7	21
66	Theoretical study of hydrogen adsorption on FePd face-centered cubic alloy surfaces. *Physical Review B*, **2005**, 71,	3.3	20
65	Synthesis and Characterization of Silver Nanoparticles Prepared with Honey: The Role of Carbohydrates. *Analytical Letters*, **2017**, 50, 877-888	2.2	19
64	The effect of interstitial hydrogen on the electronic structure of FePd alloys. *Journal of Physics and Chemistry of Solids*, **2004**, 65, 1799-1807	3.9	18
63	A van der Waals DFT study of PtH 2 systems absorbed on pristine and defective graphene. *Applied Surface Science*, **2016**, 382, 80-87	6.7	18
62	A Theoretical Study of the Effect of Zr-, Nb-Doped and Vacancy-like Defects on H Desorption on MgH2 (110) Surface. *Journal of Physical Chemistry C*, **2014**, 118, 4231-4237	3.8	17
61	Redox behavior of a low-doped Pr-CeO2(111) surface. A DFT+U study. *Applied Surface Science*, **2017**, 401, 206-217	6.7	15
60	Geometrical and Electronic Properties of Hydrated Sodium Montmorillonite and Tetracycline Montmorillonite from DFT Calculations. *Journal of Physical Chemistry C*, **2015**, 119, 16082-16088	3.8	15
59	A DFT study of phenol adsorption on a low doping MnCe composite oxide model. *Applied Surface Science*, **2015**, 359, 14-20	6.7	13
58	Density functional theory study of water interactions on Mn-doped CeO2(1 1 1) surface. *Applied Surface Science*, **2014**, 313, 784-793	6.7	13
57	Benzene and carbon monoxide co-adsorption on Pt(1 1 1): a theoretical study. *Applied Surface Science*, **2004**, 236, 394-405	6.7	13
56	Detection of oxytetracycline in honey using SERS on silver nanoparticles. *TrAC - Trends in Analytical Chemistry*, **2019**, 121, 115673	14.6	12
55	Theoretical study of the role of the interface of Ag4 nanoclusters deposited on TiO2(110) and TiO2(101). *Applied Surface Science*, **2019**, 490, 343-351	6.7	12
54	Oxygen vacancy formation on the Ni/Ce0.75Zr0.25O2(111) surface. A DFT+U study. *International Journal of Hydrogen Energy*, **2012**, 37, 14937-14944	6.7	12
53	The adsorption of CO on potassium doped molybdenum carbide surface: An ab-initio study. *Catalysis Today*, **2012**, 181, 102-107	5.3	12
52	A DFT study of hydrogen storage in Zr(Cr 0.5 Ni 0.5) 2 Laves phase. *International Journal of Hydrogen Energy*, **2016**, 41, 2700-2710	6.7	11
51	A DFT study of dopant (Zr, Nb) and vacancies on the dehydrogenation on MgH2 (001) surface. *International Journal of Hydrogen Energy*, **2014**, 39, 1732-1739	6.7	11
50	Ultra-low concentration protein detection based on phenylalanine-Pd/SWCNT as a high sensitivity nanoreceptor.. *RSC Advances*, **2020**, 10, 2650-2660	3.7	10

49	Selenium adsorption at different coverages on Fe(1 0 0) and Fe(1 1 1): A DFT study. *Applied Surface Science*, **2014**, 315, 252-260	6.7	10
48	Rhodium clustering process on defective (8,0) SWCNT: Analysis of chemical and physical properties using density functional theory. *Applied Surface Science*, **2017**, 425, 823-832	6.7	10
47	Valley properties of doped graphene in a magnetic field. *European Physical Journal B*, **2015**, 88, 1	1.2	10
46	Surface enhancement Raman spectroscopy and density functional theory study of silver nanoparticles synthetized with d-glucose. *Journal of Raman Spectroscopy*, **2018**, 49, 1756-1764	2.3	10
45	The adsorption of acrolein on a Pt (111): A study of chemical bonding and electronic structure. *Applied Surface Science*, **2012**, 263, 79-85	6.7	9
44	Adsorption of ammonia on vanadium–antimony mixed oxides. *Applied Surface Science*, **2012**, 258, 3617-3623	6.7	9
43	The adsorption of hydrogen on face centered tetragonal FePd surfaces. *Solid State Communications*, **2004**, 131, 81-85	1.6	9
42	Planck's constant determination using a light bulb. *American Journal of Physics*, **1996**, 64, 819-821	0.7	9
41	Adsorption of bentazone and imazapyc from water by using functionalized silica: Experimental and computational analysis. *Journal of Contaminant Hydrology*, **2019**, 227, 103542	3.9	8
40	Adsorption of bentazon on CAT and CARBOPAL activated carbon: Experimental and computational study. *Applied Surface Science*, **2018**, 433, 487-501	6.7	8
39	Density functional study of He–vacancy interaction in bcc iron. *Journal of Physics Condensed Matter*, **2004**, 16, 6907-6916	1.8	8
38	Molecular dynamics simulations on interaction of ssDNA-causing DM1 with carbon and boron nitride nanotubes to inhibit the formation of CTG repeat secondary structures. *Applied Surface Science*, **2020**, 524, 146572	6.7	7
37	Benzene adsorption on PtCo(1 1 1): A DFT study. *Applied Surface Science*, **2013**, 282, 17-24	6.7	7
36	A theoretical study of cyclopentene (c-C5H8) dehydrogenation to cyclopentadienyl anion (c-C5H5) on Ni (111). *Journal of Molecular Catalysis A*, **2009**, 314, 28-34		7
35	The influence of Mg on the C adsorption on Ni(1 0 0): A DFT study. *Journal of Molecular Catalysis A*, **2010**, 315, 171-177		7
34	A DFT study of H adsorption on Pt(111) and Pt–Ru(111) surfaces. *Applied Surface Science*, **2008**, 254, 5827-5830	6.7	7
33	The hydrogen effect in the electronic structure and bonding of the B2 FeAl alloy with a Fe vacancy. *International Journal of Hydrogen Energy*, **2009**, 34, 9591-9595	6.7	6
32	ADSORPTION OF HYDROGEN ON β-Ga2O3(100): A THEORETICAL STUDY. *Surface Review and Letters*, **2007**, 14, 79-86	1.1	6

31	The effect of interstitial hydrogen on the electronic structure of the B2 FeAl alloy. *Physica Status Solidi (B): Basic Research*, **2007**, 244, 3684-3694	1.3	6
30	DFT study of ethanol adsorption on CaO(0 0 1) surface. *Applied Surface Science*, **2020**, 500, 144254	6.7	6
29	THE CO-ADSORPTION OF BENZENE ANDCOONCo(0001). *Surface Review and Letters*, **2009**, 16, 749-755	1.1	5
28	Density functional theory study of selenium adsorption on Fe(1 1 0). *Applied Surface Science*, **2011**, 257, 6878-6883	6.7	5
27	The electronic structure of vanadium antimonate. *Catalysis Today*, **2005**, 107-108, 40-45	5.3	5
26	Hydrogen storage in Zr0.9Ti0.1(Ni0.5Cr0.5-xVx)2 Laves phase, with x□=□0, 0.125, 0.25, 0.375, 0.5. A theoretical approach. *International Journal of Hydrogen Energy*, **2018**, 43, 16085-16091	6.7	4
25	DFT study of □d-glucose adsorption on single-walled carbon nanotubes decorated with platinum. A bonding analysis. *Applied Surface Science*, **2017**, 423, 542-548	6.7	4
24	A computational simulation for H-dislocated BCC Fe interaction. *Materials Chemistry and Physics*, **1998**, 55, 61-67	4.4	4
23	Theoretical study of the influence of cation vacancies on the catalytic properties of vanadium antimonate. *Applied Surface Science*, **2008**, 254, 5837-5843	6.7	4
22	Influence of functionalization, surface area and charge distribution of SBA15-based adsorbents on CO (II) and NI (II) removal from aqueous solutions. *Journal of Environmental Chemical Engineering*, **2020**, 8, 103671	6.8	4
21	Experimental and DFT Studies of Hybrid Silver/Cdots Nanoparticles. *Journal of Physical Chemistry B*, **2020**, 124, 2425-2435	3.4	3
20	The Effect of Metal□cation Vacancies on Vanadium Antimonate Surface Properties. A Theoretical Study. *Journal of Physical Chemistry C*, **2013**, 117, 20548-20556	3.8	3
19	Hydrogen and carbon interaction in a FeNi alloy with a vacancy. *Physica Status Solidi (B): Basic Research*, **2009**, 246, 1275-1285	1.3	3
18	A bonding study of CO□benzene co-adsorption on Rh(111). *Journal of Molecular Catalysis A*, **2010**, 323, 23-27		3
17	Adsorption/Oxidation of CH3OH on V2O5. A Theoretical and Experimental Study. *Adsorption Science and Technology*, **1997**, 15, 517-529	3.6	3
16	Benzene and NO on a Ru(001) surface: Electronic structure and bonding. *Applied Surface Science*, **2006**, 252, 2108-2114	6.7	3
15	THE EFFECT OF H ON THE ELECTRONIC STRUCTURE OF AN Fe(110)□Pd(100) INTERFACE. *Surface Review and Letters*, **2003**, 10, 879-888	1.1	3
14	Characterization of RuMo□SiO2 catalysts. A comparative study before and after CO hydrogenation reaction. *Journal of Materials Chemistry*, **1996**, 6, 1433-1439		3

13	Propylene Adsorption On a Nonstoichiometric VSbO4(110) Surface. *Journal of Physical Chemistry C*, **2015**, 119, 4967-4975	3.8	2
12	THE OBSERVABLE-STATE MODEL AND NONRENORMALIZABLE THEORIES. *International Journal of Modern Physics A*, **2013**, 28, 1350016	1.2	2
11	The Electronic Structure and Bonding of MAO on the SiO2 (111) Hydrated Surface. *Macromolecular Theory and Simulations*, **2001**, 10, 485-490	1.5	2
10	Zirconocene interaction with MAO on (111) and (100) silica surfaces. *Macromolecular Theory and Simulations*, **2000**, 9, 381-387	1.5	2
9	A theoretic study of the indene adsorption on SiO2 surfaces. *Computational Materials Science*, **2000**, 17, 61-72	3.2	2
8	Analytic solution for gauged Dirac-Weyl equation in (2 + 1)-dimensions. *Europhysics Letters*, **2017**, 118, 21001	1.6	1
7	Zero energy mode for an electron in graphene in a perpendicular magnetic field with constant asymptotics. *Physica E: Low-Dimensional Systems and Nanostructures*, **2019**, 109, 225-227	3	1
6	A DFT study of cyclopropane adsorption on Pt(1 1 1). Electronic structure and bonding. *Applied Surface Science*, **2014**, 303, 324-330	6.7	1
5	A computer-aided modelling analogue for lattice dynamics. *European Journal of Physics*, **1997**, 18, 398-403	0.8	1
4	CO on Pd(100)/SiO2: a computational study of the effect of CaO on the energetics of adsorption. *Computational Materials Science*, **2000**, 18, 39-47	3.2	1
3	Advanced materials for hydrogen storage based on iron-palladium intermetallic alloys. *Inorganic Materials: Applied Research*, **2011**, 2, 172-175	0.6	0
2	The effect of carbon on the electronic structure of FeNi alloys with a stacking fault. *Physica Status Solidi (B): Basic Research*, **2008**, 245, 2771-2778	1.3	0
1	Theoretical study of the octahedral substitution effect in delaminated pyrophyllite: physicochemical properties and applications. *Physical Chemistry Chemical Physics*, **2021**, 23, 14601-14607	3.6	