Alfredo Juan

List of Publications by Year
in descending order

85 papers	1,408 citations	304602 22 h-index	395590 33 g-index
86 all docs	86 docs citations	86 times ranked	1755 citing authors

#	Article	IF	Citations
1	DFT Study of Hydrogen Adsorption on Palladium Decorated Graphene. Journal of Physical Chemistry C, 2011, 115, 4315-4323.	1.5	135
2	Hydrogen on the Fe(110) surface and near bulk bcc Fe vacancies. Surface Science, 1999, 421, 1-16.	0.8	72
3	Mn-Doped CeO₂: DFT+U Study of a Catalyst for Oxidation Reactions. Journal of Physical Chemistry C, 2013, 117, 18063-18073.	1.5	68
4	Hydrogen adsorption on Î²-Ga2O3(100) surface containing oxygen vacancies. Surface Science, 2005, 575, 171-180.	0.8	49
5	Theoretical Study of Hydrogen Adsorption on Ru-Decorated (8,0) Single-Walled Carbon Nanotube. Journal of Physical Chemistry C, 2014, 118, 27672-27680.	1.5	43
6	DFT study of Rh-decorated pristine, B-doped and vacancy defected graphene for hydrogen adsorption. RSC Advances, 2016, 6, 83926-83941.	1.7	39
7	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.	1.6	39
8	A theoretical study of the electronic structure and bonding of the monoclinic phase of Mg2NiH4Mg2NiH4. International Journal of Hydrogen Energy, 2007, 32, 4943-4948.	3.8	38
9	Ruthenium decorated single walled carbon nanotube for molecular hydrogen storage: A first-principle study. International Journal of Hydrogen Energy, 2019, 44, 8376-8383.	3.8	36
10	DFT study of H2 adsorption on Pd-decorated single walled carbon nanotubes with C-vacancies. International Journal of Hydrogen Energy, 2012, 37, 10156-10164.	3.8	34
11	Catalytic oxidation of CH3OH to HCOOCH3 on V2O5: A theoretical study. Journal of Molecular Catalysis A, 1997, 118, 283-291.	4.8	29
12	Preparation and characterization of Î³-Al2O3-supported Pd Mo catalysts. Applied Catalysis B: Environmental, 1998, 15, 115-127.	10.8	29
13	A First-Principles Modeling of Ni Interactions on CeO₂â^'ZrO₂Mixed Oxide Solid Solutions. Journal of Physical Chemistry C, 2011, 115, 7456-7465.	1.5	28
14	A van der Waals DFT study of PtH 2 systems absorbed on pristine and defective graphene. Applied Surface Science, 2016, 382, 80-87.	3.1	27
15	Synthesis and Characterization of Silver Nanoparticles Prepared with Honey: The Role of Carbohydrates. Analytical Letters, 2017, 50, 877-888.	1.0	27
16	Effects of potassium on the adsorption of methanol on Î²-Mo2C(001) surface. Surface Science, 2010, 604, 914-919.	0.8	26
17	Theoretical Model for CO Adsorption and Dissociation on Clean and K-Doped Î²-Mo₂C Surfaces. Journal of Physical Chemistry C, 2012, 116, 24573-24581.	1.5	26
18	Ultrathin (001) and (100) TiO2(B) sheets: Surface reactivity and structural properties. Applied Surface Science, 2014, 290, 180-187.	3.1	26

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19	Detection of oxytetracycline in honey using SERS on silver nanoparticles. TrAC - Trends in Analytical Chemistry, 2019, 121, 115673.	5.8	26
20	DFT study of ethanol adsorption on CaO(0â€¯0â€¯1) surface. Applied Surface Science, 2020, 500, 144254.	3.1	25
21	Theoretical study of hydrogen adsorption on FePd face-centered cubic alloy surfaces. Physical Review B, 2005, 71, .	1.1	24
22	The Co-adsorption of tetramethylpiperidine and TiCl4 on Î²-MgCl2. A theoretical study of a Ziegler-Natta pre-catalyst. Journal of Molecular Catalysis A, 1997, 122, 25-37.	4.8	23
23	Bonding in PdH2 and Pd2H2 systems adsorbed on carbon nanotubes: Implications for hydrogen storage. International Journal of Hydrogen Energy, 2014, 39, 8780-8790.	3.8	23
24	The effect of interstitial hydrogen on the electronic structure of Feâ€“Pd alloys. Journal of Physics and Chemistry of Solids, 2004, 65, 1799-1807.	1.9	22
25	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.	1.5	22
26	Redox behavior of a low-doped Pr-CeO2(111) surface. A DFT+U study. Applied Surface Science, 2017, 401, 206-217.	3.1	22
27	Geometrical and Electronic Properties of Hydrated Sodium Montmorillonite and Tetracycline Montmorillonite from DFT Calculations. Journal of Physical Chemistry C, 2015, 119, 16082-16088.	1.5	19
28	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.	3.8	19
29	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.	3.8	18
30	Ultra-low concentration protein detection based on phenylalanineâ€“Pd/SWCNT as a high sensitivity nanoreceptor. RSC Advances, 2020, 10, 2650-2660.	1.7	18
31	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.	3.1	17
32	Density functional theory study of water interactions on Mn-doped CeO2(111) surface. Applied Surface Science, 2014, 313, 784-793.	3.1	16
33	Oxygen vacancy formation on the Ni/Ce0.75Zr0.25O2(111) surface. A DFT+U study. International Journal of Hydrogen Energy, 2012, 37, 14937-14944.	3.8	15
34	A DFT study of phenol adsorption on a low doping Mnâ€“Ce composite oxide model. Applied Surface Science, 2015, 359, 14-20.	3.1	15
35	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.	3.1	15
36	Benzene and carbon monoxide co-adsorption on Pt(1 1 1): a theoretical study. Applied Surface Science, 2004, 236, 394-405.	3.1	14

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37	The adsorption of CO on potassium doped molybdenum carbide surface: An ab-initio study. Catalysis Today, 2012, 181, 102-107.	2.2	13
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.	3.1	13
39	Planckâ€™s constant determination using a light bulb. American Journal of Physics, 1996, 64, 819-821.	0.3	12
40	Density functional study of Hâ€“Fe vacancy interaction in bcc iron. Journal of Physics Condensed Matter, 2004, 16, 6907-6916.	0.7	11
41	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.	3.1	11
42	Adsorption of bentazone and imazapyc from water by using functionalized silica: Experimental and computational analysis. Journal of Contaminant Hydrology, 2019, 227, 103542.	1.6	11
43	The adsorption of hydrogen on face centered tetragonal FePd surfaces. Solid State Communications, 2004, 131, 81-85.	0.9	10
44	Adsorption of ammonia on vanadiumâ€“antimony mixed oxides. Applied Surface Science, 2012, 258, 3617-3623.	3.1	10
45	Valley properties of doped graphene in a magnetic field. European Physical Journal B, 2015, 88, 1.	0.6	10
46	Surface enhancement Raman spectroscopy and density functional theory study of silver nanoparticles synthetized with ‹scp›d‹/scp›â€glucose. Journal of Raman Spectroscopy, 2018, 49, 1756-1764.	1.2	10
47	Hydrogen storage in Zr0.9Ti0.1(Ni0.5Cr0.5-xVx)2 Laves phase, with xÂ=ÂO, 0.125, 0.25, 0.375, 0.5. A theoretical approach. International Journal of Hydrogen Energy, 2018, 43, 16085-16091.	3.8	10
48	Experimental and DFT Studies of Hybrid Silver/Cdots Nanoparticles. Journal of Physical Chemistry B, 2020, 124, 2425-2435.	1.2	10
49	The adsorption of acrolein on a Pt (1 1 1): A study of chemical bonding and electronic structure. Applied Surface Science, 2012, 263, 79-85.	3.1	9
50	Adsorption of bentazon on CAT and CARBOPAL activated carbon: Experimental and computational study. Applied Surface Science, 2018, 433, 487-501.	3.1	9
51	ADSORPTION OF HYDROGEN ON Î²-Ga2O3(100): A THEORETICAL STUDY. Surface Review and Letters, 2007, 14, 79-86.	0.5	8
52	The effect of interstitial hydrogen on the electronic structure of the B2 FeAl alloy. Physica Status Solidi (B): Basic Research, 2007, 244, 3684-3694.	0.7	8
53	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.	3.8	8
54	A theoretical study of cyclopentene (c-C5H8) dehydrogenation to cyclopentadienyl anion (c-C5H5â^) on Ni (111). Journal of Molecular Catalysis A, 2009, 314, 28-34.	4.8	8

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55	A DFT study of H adsorption on Pt(111) and Ptâ€“Ru(111) surfaces. Applied Surface Science, 2008, 254, 5827-5830.	3.1	7
56	The influence of Mg on the C adsorption on Ni(100): A DFT study. Journal of Molecular Catalysis A, 2010, 315, 171-177.	4.8	7
57	Benzene adsorption on PtCo(111): A DFT study. Applied Surface Science, 2013, 282, 17-24.	3.1	7
58	DFT study of Î²-d-glucose adsorption on single-walled carbon nanotubes decorated with platinum. A bonding analysis. Applied Surface Science, 2017, 423, 542-548.	3.1	7
59	The electronic structure of vanadium antimonate. Catalysis Today, 2005, 107-108, 40-45.	2.2	6
60	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.	3.3	6
61	THE CO-ADSORPTION OF BENZENE ANDCOONCo(0001). Surface Review and Letters, 2009, 16, 749-755.	0.5	5
62	Density functional theory study of selenium adsorption on Fe(110). Applied Surface Science, 2011, 257, 6878-6883.	3.1	5
63	A computational simulation for H-dislocated BCC Fe interaction. Materials Chemistry and Physics, 1998, 55, 61-67.	2.0	4
64	Theoretical study of the influence of cation vacancies on the catalytic properties of vanadium antimonate. Applied Surface Science, 2008, 254, 5837-5843.	3.1	4
65	The Effect of Metalâ€“Cation Vacancies on Vanadium Antimonate Surface Properties. A Theoretical Study. Journal of Physical Chemistry C, 2013, 117, 20548-20556.	1.5	4
66	Characterization of RuMoâ€“SiO2catalysts. A comparative study before and after CO hydrogenation reaction. Journal of Materials Chemistry, 1996, 6, 1433-1439.	6.7	3
67	Adsorption/Oxidation of CH₃OH on V₂O₅. A Theoretical and Experimental Study. Adsorption Science and Technology, 1997, 15, 517-529.	1.5	3
68	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.	1.4	3
69	THE EFFECT OF H ON THE ELECTRONIC STRUCTURE OF AN Fe(110)â€“Pd(100) INTERFACE. Surface Review and Letters, 2003, 10, 879-888.	0.5	3
70	Benzene and NO on a Ru(001) surface: Electronic structure and bonding. Applied Surface Science, 2006, 252, 2108-2114.	3.1	3
71	Hydrogen and carbon interaction in a FeNi alloy with a vacancy. Physica Status Solidi (B): Basic Research, 2009, 246, 1275-1285.	0.7	3
72	A bonding study of COâ€“benzene co-adsorption on Rh(111). Journal of Molecular Catalysis A, 2010, 323, 23-27.	4.8	3

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73	A computer-aided modelling analogue for lattice dynamics. European Journal of Physics, 1997, 18, 398-403.	0.3	2
74	Zirconocene interaction with MAO on (111) and (100) silica surfaces. Macromolecular Theory and Simulations, 2000, 9, 381-387.	0.6	2
75	A theoretic study of the indene adsorption on SiO2 surfaces. Computational Materials Science, 2000, 17, 61-72.	1.4	2
76	The Electronic Structure and Bonding of MAO on the SiO2 (111) Hydrated Surface. Macromolecular Theory and Simulations, 2001, 10, 485-490.	0.6	2
77	Advanced materials for hydrogen storage based on iron-palladium intermetallic alloys. Inorganic Materials: Applied Research, 2011, 2, 172-175.	0.1	2
78	THE OBSERVABLE-STATE MODEL AND NONRENORMALIZABLE THEORIES. International Journal of Modern Physics A, 2013, 28, 1350016.	0.5	2
79	Propylene Adsorption On a Nonstoichiometric VSbO₄(110) Surface. Journal of Physical Chemistry C, 2015, 119, 4967-4975.	1.5	2
80	Theoretical study of the octahedral substitution effect in delaminated pyrophyllite: physicochemical properties and applications. Physical Chemistry Chemical Physics, 2021, 23, 14601-14607.	1.3	2
81	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.	0.7	1
82	A DFT study of cyclopropane adsorption on Pt(111). Electronic structure and bonding. Applied Surface Science, 2014, 303, 324-330.	3.1	1
83	Analytic solution for gauged Dirac-Weyl equation in (2 + 1)-dimensions. Europhysics Letters, 2017, 118, 21001.	0.7	1
84	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.	1.3	1
85	KINETIC ANALYSIS OF SECONDARY PRECIPITATION IN A HP40-Nb ALLOY. Acta Metallurgica Slovaca, 2019, 25, 223-229.	0.3	0