

# Pedro L De Andres

## List of Publications by Year in descending order

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104  
papers

3,171  
citations

147801

31  
h-index

161849

54  
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104  
all docs

104  
docs citations

104  
times ranked

3352  
citing authors

#	ARTICLE	IF	CITATIONS
1	General Model for Water Monomer Adsorption on Close-Packed Transition and Noble Metal Surfaces. Physical Review Letters, 2003, 90, 216102.	7.8	358
2	Holographic LEED. Physical Review Letters, 1990, 64, 1270-1273.	7.8	167
3	Strong covalent bonding between two graphene layers. Physical Review B, 2008, 77, .	3.2	147
4	A diffuse LEED study of the adsorption structure of disordered benzene on Pt(111). Surface Science, 1991, 249, 21-34.	1.9	139
5	Water Dimer Diffusion on Pd{111} Assisted by an H-Bond Donor-Acceptor Tunneling Exchange. Physical Review Letters, 2004, 92, 136104.	7.8	114
6	Theory of the scanning tunneling microscope: Xe on Ni and Al. Physical Review B, 1996, 54, 2225-2235.	3.2	100
7	Bending modes, anharmonic effects, and thermal expansion coefficient in single-layer and multilayer graphene. Physical Review B, 2012, 86, .	3.2	99
8	Adsorption and reaction of CO <sub>2</sub> on Ni{110}: X-ray photoemission, near-edge X-ray absorption fine-structure and diffuse leed studies. Surface Science, 1988, 206, 1-19.	1.9	89
9	Epitaxial growth of cobalt films on Cu(100): a crystallographic LEED determination. Journal of Physics Condensed Matter, 1993, 5, 2055-2062.	1.8	80
10	Hydrogen on graphene under stress: Molecular dissociation and gap opening. Physical Review B, 2010, 81, .	3.2	77
11	Ordered Vacancy Network Induced by the Growth of Epitaxial Graphene on Pt(111). Physical Review Letters, 2010, 105, 216102.	7.8	70
12	Lifetime in a two-dimensional image-potential-induced electron band. Physical Review B, 1987, 35, 4529-4532.	3.2	69
13	Hydrogen in $\pm$ -iron: Stress and diffusion. Physical Review B, 2008, 78, .	3.2	67
14	Structure of Rutile TiO <sub>2</sub> (110) (1 Å <sup>-2</sup> ): Formation of Ti <sub>2</sub> O <sub>3</sub> Quasi-1D Metallic Chains. Physical Review Letters, 2006, 96, 055502.	7.8	60
15	Adsorbate induced reconstruction phase p(2 Å <sup>-2</sup> )O/Ni(100). Surface Science, 1990, 225, 242-248.	1.9	58
16	Elastic Scattering and the Lateral Resolution of Ballistic Electron Emission Microscopy: Focusing Effects on the Au/Si Interface. Physical Review Letters, 1996, 76, 807-810.	7.8	58
17	Crystal structure and charge-transport properties of N-trimethyltriindole: Novel p-type organic semiconductor single crystals. Organic Electronics, 2009, 10, 643-652.	2.6	56
18	Density functional theory study of the interaction of monomeric water with the Ag{111} surface. Physical Review B, 2004, 69, .	3.2	53

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19	First-principles calculation of the effect of stress on the chemical activity of graphene. Applied Physics Letters, 2008, 93, .	3.3	50
20	Calculation of the lifetimes for intermediate Rydberg states. Physical Review B, 1989, 39, 10356-10358.	3.2	47
21	<i>Ab initio</i> molecular dynamics simulation of hydrogen diffusion in $\text{Fe}_2\text{O}_3$ -iron. Physical Review B, 2010, 81, .	3.2	46
22	Crystal structure and electronic states of tripotassium picene. Physical Review B, 2011, 83, .	3.2	45
23	Blue shift of the dipolar plasma resonance in small silver particles on an alumina surface. Physical Review B, 1986, 33, 2828-2830.	3.2	44
24	Theory of ballistic electron emission microscopy. Progress in Surface Science, 2001, 66, 3-51.	8.3	43
25	On-Surface Hydrogen-Induced Covalent Coupling of Polycyclic Aromatic Hydrocarbons via a Superhydrogenated Intermediate. Journal of the American Chemical Society, 2019, 141, 3550-3557.	13.7	40
26	Diffuse low-energy electron diffraction study of disordered O/Ni(100). Physical Review B, 1988, 38, 12277-12282.	3.2	39
27	First-principles study of $\text{H}_2\text{O}$ diffusion on a metal surface: $\text{H}_2\text{O}$ on Al(100). Physical Review B, 2004, 69, .	3.2	39
28	Interplay between Fast Diffusion and Molecular Interaction in the Formation of Self-Assembled Nanostructures of <i>S</i> -Cysteine on Au(111). Langmuir, 2010, 26, 4113-4118.	3.5	38
29	<i>Ab initio</i> electronic and geometrical structures of tripotassium-intercalated phenanthrene. Physical Review B, 2011, 84, .	3.2	34
30	Understanding atomic-resolved STM images on $\text{TiO}_2(110)-(1 \times 1)$ surface by DFT calculations. Nanotechnology, 2010, 21, 405702.	2.6	33
31	Crystallography of epitaxial face centered tetragonal Co/Cu(100) by low energy electron diffraction. Journal of Magnetism and Magnetic Materials, 1993, 121, 65-68.	2.3	31
32	Hot-electron lifetimes in metals: a combined <i>ab initio</i> calculation and ballistic electron emission spectroscopy analysis. Physical Review B, 2003, 68, .	3.2	29
33	Transport of physisorbed Xe atoms on Ni(110) using a scanning tunneling microscope: A theoretical approach. Physical Review B, 1992, 45, 8721-8729.	3.2	28
34	Structural and compositional reversible phase transitions on low-index $\text{Fe}_3\text{Si}$ surfaces. Europhysics Letters, 2001, 56, 822-828.	2.0	28
35	LEED-IV study of the rutile $\text{TiO}_2(110)-(1 \times 2)$ surface with a Ti-interstitial added-row reconstruction. Physical Review B, 2007, 75, .	3.2	27
36	Graphene growth on Pt(111) and Au(111) using a MBE carbon solid-source. Diamond and Related Materials, 2015, 57, 58-62.	3.9	27

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37	Structural determination of two-dimensional $\text{YSi}_2$ epitaxially grown on Si(111). Physical Review B, 2002, 66, .	3.2	26
38	Weakly Interacting Molecular Layer of Spinning $\text{C}_{60}$ Molecules on $\text{TiO}_2$ (110) Surfaces. Chemistry - A European Journal, 2012, 18, 7382-7387.	3.3	26
39	Direct reconstruction of three-dimensional atomic adsorption sites by holographic LEED. Physical Review B, 1996, 54, 8172-8176.	3.2	25
40	Holographic reconstruction from measured diffuse low-energy-electron-diffraction intensities. Physical Review B, 1992, 45, 9402-9405.	3.2	22
41	Characterization of thin silicon overlayers on rutile $\text{TiO}_2$ . Physical Review B, 2010, 82, .	3.2	22
42	Phonon scattering in diffuse leed. Surface Science, 1988, 193, 1-9.	1.9	21
43	Electron energy relaxation times from ballistic-electron-emission spectroscopy. Physical Review B, 2000, 61, 4522-4525.	3.2	21
44	A molecular T-matrix approach to calculating Low-Energy Electron Diffraction intensities for ordered molecular adsorbates. Surface Science, 2005, 579, 89-99.	1.9	20
45	Diffusion of Hydrogen in Pd Assisted by Inelastic Ballistic Hot Electrons. Physical Review Letters, 2012, 108, 115902.	7.8	19
46	Valence band electronic structure characterization of the rutile $\text{TiO}_2$ (110)-(1 $\bar{1}$ -2) reconstructed surface. Surface Science, 2013, 608, 92-96.	1.9	19
47	A Barrier Potential Calculation for Tunneling Electrons at a Metal-Metal Interface. Europhysics Letters, 1987, 3, 101-106.	2.0	18
48	Trapping of electrons near chemisorbed hydrogen on graphene. Physical Review B, 2010, 81, .	3.2	18
49	Relaxation-time effects in the transverse dielectric function and the electromagnetic properties of metallic surfaces and small particles. Physical Review B, 1986, 34, 7365-7366.	3.2	17
50	Detecting stacking faults during epitaxial growth by low energy electron diffraction. Surface Science, 1996, 345, 320-330.	1.9	16
51	Ballistic Electron Emission Microscopy on $\text{CoSi}_2/\text{Si}(111)$ Interfaces: Band Structure Induced Atomic-Scale Resolution and Role of Localized Surface States. Physical Review Letters, 1998, 81, 4963-4966.	7.8	16
52	Quantum-mechanical analysis of the elastic propagation of electrons in the Au/Si system: Application to ballistic-electron-emission microscopy. Physical Review B, 1998, 58, 14036-14046.	3.2	16
53	Adsorption of xenon on metals: a theoretical analysis. Surface Science, 1994, 307-309, 704-709.	1.9	15
54	Adsorption of noble gases on metal surfaces and the scanning tunneling microscope. Progress in Surface Science, 1995, 48, 27-38.	8.3	15

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55	<i>Ab initio</i> study of the cubic-to-hexagonal phase transition promoted by interstitial hydrogen in iron. <i>Physical Review B</i> , 2011, 84, .	3.2	15
56	Surface atomic structure determination of three-dimensional yttrium silicide epitaxially grown on Si(111). <i>Physical Review B</i> , 2005, 71, .	3.2	14
57	One-dimensional potential for image-potential states on graphene. <i>New Journal of Physics</i> , 2014, 16, 023012.	2.9	13
58	Onâ€œSurface Bottomâ€œUp Synthesis of Azine Derivatives Displaying Strong Acceptor Behavior. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 8582-8586.	13.8	13
59	Ortho and Para Hydrogen Dimers on G/SiC(0001): Combined STM and DFT Study. <i>Langmuir</i> , 2015, 31, 233-239.	3.5	12
60	Hot electron transport in Ballistic Electron Emission Spectroscopy: Band structure effects and k parallel -space currents. <i>Europhysics Letters</i> , 1999, 45, 181-187.	2.0	11
61	Advances in direct methods in LEED: the diffuse LEED pattern as a hologram. <i>Surface Science</i> , 1992, 269-270, 1-6.	1.9	10
62	A theoretical analysis of ballistic electron emission microscopy: k-space distributions and spectroscopy. <i>Applied Surface Science</i> , 1998, 123-124, 199-206.	6.1	10
63	Diffusion and trapping of hydrogen in carbon steel at different temperatures. <i>Theoretical and Applied Fracture Mechanics</i> , 2020, 110, 102803.	4.7	10
64	Quantum size and nonlocal effects in the electromagnetic properties of small metallic spheres. <i>Physical Review B</i> , 1985, 32, 7878-7889.	3.2	9
65	Etching of Graphene in a Hydrogen-rich Atmosphere toward the Formation of Hydrocarbons in Circumstellar Clouds. <i>Journal of Physical Chemistry C</i> , 2014, 118, 26882-26886.	3.1	9
66	Quantum-size effects in the electromagnetic response of small spheres. <i>Journal of Physics C: Solid State Physics</i> , 1985, 18, 4951-4956.	1.5	8
67	A Transport Analysis of the BEEM Spectroscopy of Au/Si Schottky Barriers. <i>Physica Status Solidi (B): Basic Research</i> , 1997, 204, 397-399.	1.5	8
68	Anisotropic and anharmonic effects through the t-matrix for Low-Energy Electron Diffraction (TMAT) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	3.3	8
69	Electronic transport on Au/Si structures: Electron-electron, electron-phonon, and band structure effects. <i>Physical Review B</i> , 2002, 66, .	3.2	8
70	Spin alignment of extra electrons in K-phenanthrene clusters taken from the crystalline tripotassium-intercalated phenanthrene structure. <i>Physical Review B</i> , 2012, 85, .	3.2	8
71	Role of the Anchored Groups in the Bonding and Self-Organization of Macrocycles: Carboxylic versus Pyrrole Groups. <i>Journal of Physical Chemistry C</i> , 2013, 117, 7661-7668.	3.1	8
72	Surface and bulk band-structure effects on CoSi <sub>2</sub> /Si(111) ballistic-electron emission experiments. <i>Physical Review B</i> , 2001, 63, .	3.2	7

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73	Patterson function from low-energy electron diffraction measured intensities and structural discrimination. <i>Physical Review B</i> , 2003, 67, .	3.2	7
74	Metal-catalyst-free gas-phase synthesis of long-chain hydrocarbons. <i>Nature Communications</i> , 2021, 12, 5937.	12.8	7
75	A LEED study of $c(2\sqrt{2}\times 2)$ Cu and Ag/Mo(100). <i>Surface Science</i> , 1992, 269-270, 713-718.	1.9	6
76	Surface diffraction structure determination from combinatorial simultaneous optimization. <i>Surface Science</i> , 2006, 600, L91-L95.	1.9	6
77	Multiscale modeling of Schottky-barrier MOSFETs with disilicide source/drain contacts: Role of contacts in the carrier injection. <i>Physical Review B</i> , 2007, 76, .	3.2	6
78	Monitoring and Forecasting COVID-19: Heuristic Regression, Susceptible-Infected-Removed Model and, Spatial Stochastic. <i>Frontiers in Applied Mathematics and Statistics</i> , 2021, 7, 650716.	1.3	6
79	Manifestation of Quantum Chaos in Scattering Techniques: Application to Low-Energy and Photoelectron Diffraction Intensities. <i>Physical Review Letters</i> , 1998, 80, 980-983.	7.8	5
80	A comparison between BEEM currents on Au/Si(1 1 1) and Au/Si(1 0 0): inelastic and geometrical effects. <i>Surface Science</i> , 2001, 482-485, 430-436.	1.9	5
81	Hydrogen in $\delta$ -iron: role of phonons in the diffusion of interstitials at high temperature. <i>Scientific Reports</i> , 2019, 9, 12127.	3.3	5
82	On-Surface Driven Formal Michael Addition Produces $m$ -Polyaniline Oligomers on Pt(111). <i>Angewandte Chemie - International Edition</i> , 2020, 59, 23220-23227.	13.8	5
83	Electronic surface structure of CoSi <sub>2</sub> (111)/Si(111): implications for ballistic electron-emission microscopy currents. <i>Applied Surface Science</i> , 2000, 166, 103-107.	6.1	4
84	Cálculo de la velocidad de propagación de la fisura debido a fragilización por hidrógeno. <i>Hormigon Y Acero</i> , 2016, 67, 325-332.	0.2	4
85	Effects of Li Confined Motion on NMR Quadrupolar Interactions: A Combined <sup>7</sup> Li NMR and DFT+DM Study of LiR <sub>2</sub> (PO <sub>4</sub> ) <sub>3</sub> (R=Ti or Zr) Phases. <i>ChemSusChem</i> , 2020, 13, 1027-1036.	6.8	4
86	Macroscopic Versus Microscopic Schottky Barrier Determination at (Au/Pt)/Ge(100): Interfacial Local Modulation. <i>ACS Applied Materials &amp; Interfaces</i> , 2020, 12, 28894-28902.	8.0	4
87	Surface photoeffect with non specular surface scattering of electrons. <i>Journal De Physique</i> , 1982, 43, 685-689.	1.8	4
88	Quantum chaos on ordered structures by scattering techniques: Application to low-energy electron diffraction. <i>Physical Review B</i> , 1999, 59, 3086-3094.	3.2	3
89	Green's function calculation of Ballistic Electron Emission Microscopy currents (BEEM v2.1). <i>Computer Physics Communications</i> , 2000, 127, 327-342.	7.5	3
90	A FORTRAN-90 Low-Energy Electron Diffraction program (LEED90 v1.1). <i>Computer Physics Communications</i> , 2004, 161, 151-165.	7.5	3

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91	Molecular t-matrices for Low-Energy Electron Diffraction (TMOL v1.1). Computer Physics Communications, 2004, 161, 166-178.	7.5	3
92	Quantitative LEED analysis using a simultaneous optimization algorithm. Journal of Physics Condensed Matter, 2008, 20, 304201.	1.8	3
93	Hydrogen Embrittlement of High Strength Steels. Defect and Diffusion Forum, 0, 289-292, 203-209.	0.4	3
94	Electron transport in ultra-thin films and ballistic electron emission microscopy. Journal of Physics Condensed Matter, 2017, 29, 115001.	1.8	3
95	Electromagnetic properties of small metallic spheres: Diffuse surface scattering. Physical Review B, 1986, 34, 2886-2888.	3.2	2
96	Recent Advances in Diffuse LEED as a Surface Structure Tool. Physica Scripta, 1991, T39, 318-322.	2.5	2
97	Schottky-barrier formation at passivated surfaces: covalent and ionic semiconductors. Applied Surface Science, 1996, 104-105, 183-187.	6.1	2
98	The transport and switching of Xe atoms on the Ni-W interface of a scanning tunnelling microscope. Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics, 1993, 15, 451-457.	0.4	1
99	Fast first-order perturbation approach to the surface structural problem using low energy electron diffraction. Surface Science, 1996, 348, 197-208.	1.9	1
100	Rotation assisted diffusion of water trimers on Pd{111}. Surface Science, 2016, 648, 256-261.	1.9	1
101	Onâ€šSurface Driven Formal Michael Addition Produces m â€šPolyaniline Oligomers on Pt(111). Angewandte Chemie, 2020, 132, 23420-23427.	2.0	1
102	Density Functional Theory Modeling of Solid-State Nuclear Magnetic Resonances for Polycyclic Aromatic Hydrocarbons. Journal of Physical Chemistry C, 2018, 122, 11008-11014.	3.1	0
103	How Au Outperforms Pt in the Catalytic Reduction of Methane Towards Ethane and Molecular Hydrogen. Topics in Catalysis, 2018, 61, 1290-1299.	2.8	0
104	A Theoretical Analysis of Ballistic Electron Emission Microscopy: Band Structure Effects and Attenuation Lengths. Acta Physica Polonica A, 1998, 93, 281-287.	0.5	0