Isabel LÃ³pez TocÃ³n

List of Publications by Year
in descending order

67 papers	1,837 citations	236925 25 h-index	276875 41 g-index
67 all docs	67 docs citations	67 times ranked	1556 citing authors

#	Article	IF	Citations
1	The role of charge-transfer states of the metal-adsorbate complex in surface-enhanced Raman scattering. Journal of Chemical Physics, 2002, 116, 7207-7216.	3.0	122
2	Charge Transfer Processes in Surface-Enhanced Raman Scattering. Franckâ"Condon Active Vibrations of Pyridine. The Journal of Physical Chemistry, 1996, 100, 9254-9261.	2.9	120
3	Complete analysis of the surface-enhanced Raman scattering of pyrazine on the silver electrode on the basis of a resonant charge transfer mechanism involving three states. Journal of Chemical Physics, 2000, 112, 7669-7683.	3.0	110
4	Vibrational spectrum of 3-methyl and 4-methylpyridine. Journal of Molecular Structure, 1998, 470, 241-246.	3.6	74
5	Vibrational spectra of methylpyridines. Journal of Molecular Structure, 1999, 476, 139-150.	3.6	64
6	Multicomponent Direct Detection of Polycyclic Aromatic Hydrocarbons by Surface-Enhanced Raman Spectroscopy Using Silver Nanoparticles Functionalized with the Viologen Host Lucigenin. Analytical Chemistry, 2011, 83, 2518-2525.	6.5	64
7	A Priori Scaled Quantum Mechanical Vibrational Spectra of trans- and cis-Stilbene. The Journal of Physical Chemistry, 1995, 99, 11392-11398.	2.9	62
8	Carbene Formation in Its Lower Singlet State from Photoexcited 3H-Diazirine or Diazomethane. A Combined CASPT2 and ab Initio Direct Dynamics Trajectory Study. Journal of the American Chemical Society, 2002, 124, 1728-1735.	13.7	57
9	Vibrational study of the metalâ€"adsorbate interaction of phenylacetic acid and Î±-phenylglycine on silver surfaces. Journal of Colloid and Interface Science, 2003, 263, 357-363.	9.4	57
10	Selection Rules of the Charge Transfer Mechanism of Surface-Enhanced Raman Scattering:Â The Effect of the Adsorption on the Relative Intensities of Pyrimidine Bonded to Silver Nanoclusters. Journal of Physical Chemistry B, 2006, 110, 14916-14922.	2.6	57
11	Role of the Electrode Potential in the Charge-Transfer Mechanism of Surface-Enhanced Raman Scattering. Journal of Physical Chemistry B, 2003, 107, 13143-13149.	2.6	55
12	Detection and quantitative analysis of carbendazim herbicide on Ag nanoparticles via surfaceâ€enhanced Raman scattering. Journal of Raman Spectroscopy, 2015, 46, 1095-1101.	2.5	51
13	How the electrode potential controls the selection rules of the charge transfer mechanism of SERS. Chemical Communications, 2011, 47, 4213.	4.1	50
14	Resonant charge transfer on the nanoscale: studying doublet states of adsorbates by surface-enhanced Raman scattering. Journal of Raman Spectroscopy, 2005, 36, 515-521.	2.5	44
15	Potential-energy surfaces related to the thermal decomposition of ethyl azide: The role of intersystem crossings. Journal of Chemical Physics, 2000, 113, 2282-2289.	3.0	41
16	Vibrational spectrum of 4-fluoraniline. Journal of Molecular Structure, 2001, 565-566, 421-425.	3.6	39
17	Franckâ€"Condon Dominates the Surface-Enhanced Raman Scattering of 3-Methylpyridine: Propensity Rules of the Charge-Transfer Mechanism under Reduced Symmetry. Journal of Physical Chemistry C, 2012, 116, 23639-23645.	3.1	39
18	Surface Orientation of Pyrazine Adsorbed on Silver from the Surface-Enhanced Raman Scattering Recorded at Different Electrode Potentials. Langmuir, 2002, 18, 3100-3104.	3.5	38

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19	Adsorption of carbendazim pesticide on plasmonic nanoparticles studied by surface-enhanced Raman scattering. Journal of Colloid and Interface Science, 2016, 465, 183-189.	9.4	37
20	Surface-enhanced Raman scattering of 3-phenylpropionic acid (hydrocinnamic acid). Journal of Raman Spectroscopy, 2002, 33, 455-459.	2.5	34
21	A DFT Approach to the Surface-Enhanced Raman Scattering of 4-Cyanopyridine Adsorbed on Silver Nanoparticles. Nanomaterials, 2019, 9, 1211.	4.1	33
22	DFT and CASPT2 study of two thermal reactions of nitromethane: Câ€“N bond cleavage and nitro-to-nitrite isomerization. An example of the inverse symmetry breaking deficiency in density functional calculations of an homolytic dissociation. Computational and Theoretical Chemistry, 2003, 630, 17-23.	1.5	32
23	NH2 inversion potential in the S0 and S1 electronic states of aniline: fit to the (ro-)vibrational data and comparison with ab initio and density functional results. Chemical Physics Letters, 2000, 327, 45-53.	2.6	27
24	Nitrenes as intermediates in the thermal decomposition of aliphatic azides. International Journal of Quantum Chemistry, 2001, 84, 241-248.	2.0	27
25	An MS-CASPT2 study of the photodecomposition of 4-methoxyphenyl azide: role of internal conversion and intersystem crossing. Physical Chemistry Chemical Physics, 2018, 20, 7764-7771.	2.8	26
26	Charge transfer in SERS: spectra of 3,5-dimethylpyridine at a silver electrode. Journal of Raman Spectroscopy, 1998, 29, 673-679.	2.5	25
27	The anilineâ€“water and anilineâ€“methanol complexes in the S1 excited state. Chemical Physics, 2006, 330, 138-145.	1.9	25
28	How a resonant charge transfer mechanism determines the relative intensities in the SERS spectra of 4-methylpyridine. Vibrational Spectroscopy, 2002, 29, 147-154.	2.2	23
29	Surface-enhanced Raman scattering of 5-fluorouracil adsorbed on silver nanostructures. Physical Chemistry Chemical Physics, 2009, 11, 7437.	2.8	23
30	The electronic structure of metalâ€“molecule hybrids in charged interfaces: surface-enhanced Raman selection rules derived from plasmon-like resonances. Physical Chemistry Chemical Physics, 2015, 17, 2326-2329.	2.8	21
31	The charge transfer mechanism in the SERS of 2-methylpyrazine on silver electrode. Vibrational Spectroscopy, 1999, 19, 213-221.	2.2	20
32	The anilineâ€“argon van der Waals complex: ab initio second-order MÃ¸llerâ€“Plesset study of the potential energy surface in the ground electronic state. Chemical Physics, 1999, 249, 113-120.	1.9	20
33	Selection rules for the charge transfer enhancement mechanism in SERS: dependence of the intensities on the L-matrix. Journal of Molecular Structure, 2001, 565-566, 369-372.	3.6	20
34	Trace Detection of Triphenylene by Surface Enhanced Raman Spectroscopy Using Functionalized Silver Nanoparticles with Bis-Acridinium Lucigenine. Langmuir, 2010, 26, 6977-6981.	3.5	20
35	Application of surface-enhanced resonance Raman scattering (SERS) to the study of organic functional materials: electronic structure and charge transfer properties of 9,10-bis((E)-2-(pyridin-4-yl)vinyl)anthracene. RSC Advances, 2019, 9, 14511-14519.	3.6	19
36	Inversion Motion and S1Equilibrium Geometry of 4-Fluoroaniline:Â Molecular Beam High-Resolution Spectroscopy and ab Initio Calculations. Journal of Physical Chemistry A, 1999, 103, 8946-8951.	2.5	16

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37	Vibrational spectra of cis-stilbene. Journal of Molecular Structure, 1995, 349, 29-32.	3.6	15
38	Charge transfer at the nanoscale and the role of the out-of-plane vibrations in the selection rules of surface-enhanced Raman scattering. Physical Chemistry Chemical Physics, 2018, 20, 29430-29439.	2.8	15
39	Huge Energy Gain in Metal-to-Molecule Charge Transfer Processes: A Combined Effect of an Electrical Capacitive Enhancement in Nanometer-Size Hot Spots and the Electronic Structure of the Surface Complex. Journal of Physical Chemistry C, 2014, 118, 2718-2725.	3.1	14
40	Surface-Enhanced Raman Spectroscopy for Bisphenols Detection: Toward a Better Understanding of the Analyteâ€“Nanosystem Interactions. Nanomaterials, 2021, 11, 881.	4.1	14
41	Theoretical Approaches for Modeling the Effect of the Electrode Potential in the SERS Vibrational Wavenumbers of Pyridine Adsorbed on a Charged Silver Surface. Frontiers in Chemistry, 2019, 7, 423.	3.6	13
42	Surface-enhanced Raman scattering of 2,3-dimethylpyrazine adsorbed on silver electrode: selective enhancement explained through the charge transfer mechanism. Vibrational Spectroscopy, 2004, 35, 39-44.	2.2	12
43	Synthesis of penta-p-phenylenes with oligo(ethylene glycol) side chains. Tetrahedron Letters, 2007, 48, 6075-6079.	1.4	12
44	Vibrational spectrum of 2-methylpyridine. Journal of Molecular Structure, 1997, 410-411, 443-446.	3.6	11
45	A priori SQM vibrational spectrum of 2,2â€²-bipyridine. Journal of Molecular Structure, 1997, 410-411, 447-450.	3.6	11
46	Potential coupling of intramolecular to intermolecular modes: an ab initio study of the amino inversion and van der Waals motions in the anilineâ€“argon complex. Chemical Physics, 2001, 269, 29-36.	1.9	11
47	On the dual character of charged metalâ€“molecule hybrids and the opposite behaviour of the forward and reverse CT processes. Physical Chemistry Chemical Physics, 2014, 16, 22958-22961.	2.8	11
48	Photoinduced charge transfer processes in the surface-enhanced Raman scattering of 2,4,6-trimethylpyridine recorded on silver electrode. Chemical Physics Letters, 2003, 377, 111-118.	2.6	8
49	Surface enhanced Raman scattering of trans-3-hydroxycinnamic acid adsorbed on silver nanoparticles. Chemical Physics Letters, 2008, 467, 101-104.	2.6	8
50	Raman Study of the Rigidity of Penta-p-phenylene Derivatives Used as Legs in Molecular Tripods. Journal of Physical Chemistry B, 2008, 112, 5363-5367.	2.6	8
51	Comment on â€œElucidation of charge-transfer SERS selection rules by considering the excited state properties and the role of electrode potentialâ€•by M. Mohammadpour, M. H. Khodabandeh, L. Visscher and Z. Jamshidi, Phys. Chem. Chem. Phys., 2017, 19, 7833. Physical Chemistry Chemical Physics, 2017, 19, 27888-27891.	2.8	8
52	Comparative Performance of Citrate, Borohydride, Hydroxylamine and Î²-Cyclodextrin Silver Sols for Detecting Ibuprofen and Caffeine Pollutants by Means of Surface-Enhanced Raman Spectroscopy. Nanomaterials, 2020, 10, 2339.	4.1	8
53	Building hot spots in different plasmonic nanoparticles from a cruciform bifunctional dipyridine anthracene. Journal of Raman Spectroscopy, 2019, 50, 847-855.	2.5	7
54	Moodle Quizzes as a Continuous Assessment in Higher Education: An Exploratory Approach in Physical Chemistry. Education Sciences, 2021, 11, 500.	2.6	7

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55	Large amplitude motions in the electronic ground state of 4-fluoroaniline. Physical Chemistry Chemical Physics, 2000, 2, 1351-1355.	2.8	6
56	Vibrational spectra of phenylacetate and phenylglycinate ions. Journal of Molecular Structure, 2003, 651-653, 601-606.	3.6	6
57	Intramolecular and Metal-to-Molecule Charge Transfer Electronic Resonances in the Surface-Enhanced Raman Scattering of 1,4-Bis((E)-2-(pyridin-4-yl)vinyl)naphthalene. Molecules, 2019, 24, 4622.	3.8	6
58	Proving the Dual Electronic Structure of Charged Metal-Molecule Interfaces: Surface-Enhanced Raman Scattering of Cyanide Adsorbed on a Nanostructured Silver Electrode. Journal of Physical Chemistry C, 2020, 124, 17632-17639.	3.1	6
59	Differentiated adsorption of thiobenzoic acid and thiobenzamide on silver nanoparticles determined by SERS spectroscopy. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 246, 119048.	3.9	6
60	Rotationally resolved electronic spectroscopy of aniline excited vibronic levels. Chemical Physics Letters, 2001, 335, 195-200.	2.6	5
61	Scaled quantum mechanical force field of dimethylpyrazines: vibrational assignments. Journal of Molecular Structure, 2005, 744-747, 289-293.	3.6	5
62	Vibrational predissociation dynamics of the anilineâ€“neon Van der Waals complex: an ab initio study. Chemical Physics, 2004, 303, 143-150.	1.9	4
63	High resolution electronic spectroscopy of 4-fluoroaniline in a molecular beam: new experimental results and their interpretation in terms of molecular geometry. Journal of Molecular Structure, 1999, 480-481, 269-272.	3.6	2
64	An approach to the electronic structure of molecular junctions with metal clusters of atomic thickness. Physical Chemistry Chemical Physics, 2016, 18, 27179-27184.	2.8	2
65	Voltage selection of physisorbed or chemisorbed 4-cyanobenzoate on a nanostructured silver electrode and the dual electronic structure of charged metalâ€“molecule hybrids. Applied Surface Science, 2022, 579, 152071.	6.1	2
66	Assignment of the vibrational spectrum of trimethylpyrazine. Journal of Molecular Structure, 2007, 834-836, 567-571.	3.6	1
67	Structure and Dynamics of van der Waals Complexes by High Resolution Spectroscopy. , 2001, , 393-404.		1