

Isabel LÃ³pez TocÃ¡n

List of Publications by Year in descending order

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67
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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	Voltage selection of physisorbed or chemisorbed 4-cyanobenzoate on a nanostructured silver electrode and the dual electronic structure of charged metal–molecule hybrids. <i>Applied Surface Science</i> , 2022, 579, 152071.	6.1	2
2	Differentiated adsorption of thiobenzoic acid and thiobenzamide on silver nanoparticles determined by SERS spectroscopy. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 246, 119048.	3.9	6
3	Surface-Enhanced Raman Spectroscopy for Bisphenols Detection: Toward a Better Understanding of the Analyte–Nanosystem Interactions. <i>Nanomaterials</i> , 2021, 11, 881.	4.1	14
4	Moodle Quizzes as a Continuous Assessment in Higher Education: An Exploratory Approach in Physical Chemistry. <i>Education Sciences</i> , 2021, 11, 500.	2.6	7
5	Proving the Dual Electronic Structure of Charged Metal-Molecule Interfaces: Surface-Enhanced Raman Scattering of Cyanide Adsorbed on a Nanostructured Silver Electrode. <i>Journal of Physical Chemistry C</i> , 2020, 124, 17632-17639.	3.1	6
6	Comparative Performance of Citrate, Borohydride, Hydroxylamine and β -Cyclodextrin Silver Sols for Detecting Ibuprofen and Caffeine Pollutants by Means of Surface-Enhanced Raman Spectroscopy. <i>Nanomaterials</i> , 2020, 10, 2339.	4.1	8
7	A DFT Approach to the Surface-Enhanced Raman Scattering of 4-Cyanopyridine Adsorbed on Silver Nanoparticles. <i>Nanomaterials</i> , 2019, 9, 1211.	4.1	33
8	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. <i>RSC Advances</i> , 2019, 9, 14511-14519.	3.6	19
9	Theoretical Approaches for Modeling the Effect of the Electrode Potential in the SERS Vibrational Wavenumbers of Pyridine Adsorbed on a Charged Silver Surface. <i>Frontiers in Chemistry</i> , 2019, 7, 423.	3.6	13
10	Building hot spots in different plasmonic nanoparticles from a cruciform bifunctional dipyrindine anthracene. <i>Journal of Raman Spectroscopy</i> , 2019, 50, 847-855.	2.5	7
11	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. <i>Molecules</i> , 2019, 24, 4622.	3.8	6
12	An MS-CASPT2 study of the photodecomposition of 4-methoxyphenyl azide: role of internal conversion and intersystem crossing. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 7764-7771.	2.8	26
13	Charge transfer at the nanoscale and the role of the out-of-plane vibrations in the selection rules of surface-enhanced Raman scattering. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 29430-29439.	2.8	15
14	Comment on ‘‘Elucidation of charge-transfer SERS selection rules by considering the excited state properties and the role of electrode potential’’ by M. Mohammadpour, M. H. Khodabandeh, L. Visscher and Z. Jamshidi, <i>Phys. Chem. Chem. Phys.</i> , 2017, 19, 7833. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 27888-27891.	2.8	8
15	An approach to the electronic structure of molecular junctions with metal clusters of atomic thickness. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 27179-27184.	2.8	2
16	Adsorption of carbendazim pesticide on plasmonic nanoparticles studied by surface-enhanced Raman scattering. <i>Journal of Colloid and Interface Science</i> , 2016, 465, 183-189.	9.4	37
17	Detection and quantitative analysis of carbendazim herbicide on Ag nanoparticles via surface-enhanced Raman scattering. <i>Journal of Raman Spectroscopy</i> , 2015, 46, 1095-1101.	2.5	51
18	The electronic structure of metal–molecule hybrids in charged interfaces: surface-enhanced Raman selection rules derived from plasmon-like resonances. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 2326-2329.	2.8	21

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19	On the dual character of charged metal-molecule hybrids and the opposite behaviour of the forward and reverse CT processes. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 22958-22961.	2.8	11
20	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. <i>Journal of Physical Chemistry C</i> , 2014, 118, 2718-2725.	3.1	14
21	Franck-Condon Dominates the Surface-Enhanced Raman Scattering of 3-Methylpyridine: Propensity Rules of the Charge-Transfer Mechanism under Reduced Symmetry. <i>Journal of Physical Chemistry C</i> , 2012, 116, 23639-23645.	3.1	39
22	How the electrode potential controls the selection rules of the charge transfer mechanism of SERS. <i>Chemical Communications</i> , 2011, 47, 4213.	4.1	50
23	Multicomponent Direct Detection of Polycyclic Aromatic Hydrocarbons by Surface-Enhanced Raman Spectroscopy Using Silver Nanoparticles Functionalized with the Viologen Host Lucigenin. <i>Analytical Chemistry</i> , 2011, 83, 2518-2525.	6.5	64
24	Trace Detection of Triphenylene by Surface Enhanced Raman Spectroscopy Using Functionalized Silver Nanoparticles with Bis-Acrinium Lucigenine. <i>Langmuir</i> , 2010, 26, 6977-6981.	3.5	20
25	Surface-enhanced Raman scattering of 5-fluorouracil adsorbed on silver nanostructures. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 7437.	2.8	23
26	Surface enhanced Raman scattering of trans-3-hydroxycinnamic acid adsorbed on silver nanoparticles. <i>Chemical Physics Letters</i> , 2008, 467, 101-104.	2.6	8
27	Raman Study of the Rigidity of Penta- <i>p</i> -phenylene Derivatives Used as Legs in Molecular Tripods. <i>Journal of Physical Chemistry B</i> , 2008, 112, 5363-5367.	2.6	8
28	Synthesis of penta- <i>p</i> -phenylenes with oligo(ethylene glycol) side chains. <i>Tetrahedron Letters</i> , 2007, 48, 6075-6079.	1.4	12
29	Assignment of the vibrational spectrum of trimethylpyrazine. <i>Journal of Molecular Structure</i> , 2007, 834-836, 567-571.	3.6	1
30	Selection Rules of the Charge Transfer Mechanism of Surface-Enhanced Raman Scattering: The Effect of the Adsorption on the Relative Intensities of Pyrimidine Bonded to Silver Nanoclusters. <i>Journal of Physical Chemistry B</i> , 2006, 110, 14916-14922.	2.6	57
31	The aniline-water and aniline-methanol complexes in the S1 excited state. <i>Chemical Physics</i> , 2006, 330, 138-145.	1.9	25
32	Scaled quantum mechanical force field of dimethylpyrazines: vibrational assignments. <i>Journal of Molecular Structure</i> , 2005, 744-747, 289-293.	3.6	5
33	Resonant charge transfer on the nanoscale: studying doublet states of adsorbates by surface-enhanced Raman scattering. <i>Journal of Raman Spectroscopy</i> , 2005, 36, 515-521.	2.5	44
34	Surface-enhanced Raman scattering of 2,3-dimethylpyrazine adsorbed on silver electrode: selective enhancement explained through the charge transfer mechanism. <i>Vibrational Spectroscopy</i> , 2004, 35, 39-44.	2.2	12
35	Vibrational predissociation dynamics of the aniline-neon Van der Waals complex: an ab initio study. <i>Chemical Physics</i> , 2004, 303, 143-150.	1.9	4
36	Photoinduced charge transfer processes in the surface-enhanced Raman scattering of 2,4,6-trimethylpyridine recorded on silver electrode. <i>Chemical Physics Letters</i> , 2003, 377, 111-118.	2.6	8

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37	Vibrational study of the metal-adsorbate interaction of phenylacetic acid and L-phenylglycine on silver surfaces. <i>Journal of Colloid and Interface Science</i> , 2003, 263, 357-363.	9.4	57
38	Vibrational spectra of phenylacetate and phenylglycinate ions. <i>Journal of Molecular Structure</i> , 2003, 651-653, 601-606.	3.6	6
39	DFT and CASPT2 study of two thermal reactions of nitromethane: C-N bond cleavage and nitro-to-nitrite isomerization. An example of the inverse symmetry breaking deficiency in density functional calculations of an homolytic dissociation. <i>Computational and Theoretical Chemistry</i> , 2003, 630, 17-23.	1.5	32
40	Role of the Electrode Potential in the Charge-Transfer Mechanism of Surface-Enhanced Raman Scattering. <i>Journal of Physical Chemistry B</i> , 2003, 107, 13143-13149.	2.6	55
41	The role of charge-transfer states of the metal-adsorbate complex in surface-enhanced Raman scattering. <i>Journal of Chemical Physics</i> , 2002, 116, 7207-7216.	3.0	122
42	Surface Orientation of Pyrazine Adsorbed on Silver from the Surface-Enhanced Raman Scattering Recorded at Different Electrode Potentials. <i>Langmuir</i> , 2002, 18, 3100-3104.	3.5	38
43	Carbene Formation in Its Lower Singlet State from Photoexcited 3H-Diazirine or Diazomethane. A Combined CASPT2 and ab Initio Direct Dynamics Trajectory Study. <i>Journal of the American Chemical Society</i> , 2002, 124, 1728-1735.	13.7	57
44	Surface-enhanced Raman scattering of 3-phenylpropionic acid (hydrocinnamic acid). <i>Journal of Raman Spectroscopy</i> , 2002, 33, 455-459.	2.5	34
45	How a resonant charge transfer mechanism determines the relative intensities in the SERS spectra of 4-methylpyridine. <i>Vibrational Spectroscopy</i> , 2002, 29, 147-154.	2.2	23
46	Selection rules for the charge transfer enhancement mechanism in SERS: dependence of the intensities on the L-matrix. <i>Journal of Molecular Structure</i> , 2001, 565-566, 369-372.	3.6	20
47	Vibrational spectrum of 4-fluoroaniline. <i>Journal of Molecular Structure</i> , 2001, 565-566, 421-425.	3.6	39
48	Nitrenes as intermediates in the thermal decomposition of aliphatic azides. <i>International Journal of Quantum Chemistry</i> , 2001, 84, 241-248.	2.0	27
49	Rotationally resolved electronic spectroscopy of aniline excited vibronic levels. <i>Chemical Physics Letters</i> , 2001, 335, 195-200.	2.6	5
50	Potential coupling of intramolecular to intermolecular modes: an ab initio study of the amino inversion and van der Waals motions in the aniline-argon complex. <i>Chemical Physics</i> , 2001, 269, 29-36.	1.9	11
51	Structure and Dynamics of van der Waals Complexes by High Resolution Spectroscopy. , 2001, , 393-404.		1
52	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. <i>Chemical Physics Letters</i> , 2000, 327, 45-53.	2.6	27
53	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. <i>Journal of Chemical Physics</i> , 2000, 112, 7669-7683.	3.0	110
54	Large amplitude motions in the electronic ground state of 4-fluoroaniline. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 1351-1355.	2.8	6

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55	Potential-energy surfaces related to the thermal decomposition of ethyl azide: The role of intersystem crossings. <i>Journal of Chemical Physics</i> , 2000, 113, 2282-2289.	3.0	41
56	Vibrational spectra of methylpyridines. <i>Journal of Molecular Structure</i> , 1999, 476, 139-150.	3.6	64
57	High resolution electronic spectroscopy of 4-fluoroaniline in a molecular beam: new experimental results and their interpretation in terms of molecular geometry. <i>Journal of Molecular Structure</i> , 1999, 480-481, 269-272.	3.6	2
58	The charge transfer mechanism in the SERS of 2-methylpyrazine on silver electrode. <i>Vibrational Spectroscopy</i> , 1999, 19, 213-221.	2.2	20
59	The aniline-argon van der Waals complex: ab initio second-order MÃ¶ller-Plesset study of the potential energy surface in the ground electronic state. <i>Chemical Physics</i> , 1999, 249, 113-120.	1.9	20
60	Inversion Motion and S1 Equilibrium Geometry of 4-Fluoroaniline: A Molecular Beam High-Resolution Spectroscopy and ab Initio Calculations. <i>Journal of Physical Chemistry A</i> , 1999, 103, 8946-8951.	2.5	16
61	Charge transfer in SERS: spectra of 3,5-dimethylpyridine at a silver electrode. <i>Journal of Raman Spectroscopy</i> , 1998, 29, 673-679.	2.5	25
62	Vibrational spectrum of 3-methyl and 4-methylpyridine. <i>Journal of Molecular Structure</i> , 1998, 470, 241-246.	3.6	74
63	Vibrational spectrum of 2-methylpyridine. <i>Journal of Molecular Structure</i> , 1997, 410-411, 443-446.	3.6	11
64	A priori SQM vibrational spectrum of 2,2'-bipyridine. <i>Journal of Molecular Structure</i> , 1997, 410-411, 447-450.	3.6	11
65	Charge Transfer Processes in Surface-Enhanced Raman Scattering. Franck-Condon Active Vibrations of Pyridine. <i>The Journal of Physical Chemistry</i> , 1996, 100, 9254-9261.	2.9	120
66	Vibrational spectra of cis-stilbene. <i>Journal of Molecular Structure</i> , 1995, 349, 29-32.	3.6	15
67	A Priori Scaled Quantum Mechanical Vibrational Spectra of trans- and cis-Stilbene. <i>The Journal of Physical Chemistry</i> , 1995, 99, 11392-11398.	2.9	62