JosÃ© Antonio VergÃ©s

List of Publications by Year
in descending order

50 papers	1,634 citations	394421 19 h-index	289244 40 g-index

51 all docs	51 docs citations	51 times ranked	1934 citing authors

#	Article	IF	Citations
1	Exploring the Photocyclization Pathways of Styrylthiophenes in the Synthesis of Thiahelicenes: When the Theory and Experiment Meet. Journal of Organic Chemistry, 2021, 86, 5668-5679.	3.2	5
2	Transport and Optical Gaps in Amorphous Organic Molecular Materials. Molecules, 2019, 24, 609.	3.8	0
3	Gap opening in the most stable phases of K₃ Terphenyl compound. Materials Research Express, 2019, 6, 125111.	1.6	1
4	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
5	Size-scaling behaviour of the electronic polarizability of one-dimensional interacting systems. Journal of Physics Condensed Matter, 2018, 30, 175603.	1.8	3
6	Prediction of a metallic phase for Cs3Pentacene compound. Materials Research Express, 2018, 5, 066554.	1.6	2
7	Are Electron Affinity and Ionization Potential Intrinsic Parameters to Predict the Electron or Hole Acceptor Character of Amorphous Molecular Materials?. Journal of Physical Chemistry Letters, 2017, 8, 2445-2449.	4.6	40
8	Structural and electronic changes of pentacene induced by potassium doping. Physical Review B, 2017, 95, .	3.2	4
9	Herringbone Pattern and CHâ€“Ï€ Bonding in the Crystal Architecture of Linear Polycyclic Aromatic Hydrocarbons. ChemPhysChem, 2016, 17, 3548-3557.	2.1	23
10	Can model Hamiltonians describe the electronâ€“electron interaction inÏ€-conjugated systems?: PAH and graphene. Journal of Physics Condensed Matter, 2015, 27, 463001.	1.8	10
11	On the forbidden gap of finite graphene nanoribbons. European Physical Journal B, 2015, 88, 1.	1.5	5
12	Role of potassium orbitals in the metallic behavior of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="normal">K</mml:mi><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub><mml:mi mathvariant="normal">picene</mml:mi></mml:math>. Physical Review B, 2014, 90, .	3.2	1
13	Exponential decay of spin-spin correlation between distant defect states produced by contour hydrogenation of polycyclic aromatic hydrocarbon molecules. Physical Review B, 2013, 87, .	3.2	6
14	Spin alignment of extra electrons in K-phenanthrene clusters taken from the crystalline tripotassium-intercalated phenanthrene structure. Physical Review B, 2012, 85, .	3.2	8
15	PPP Hamiltonian for polar polycyclic aromatic hydrocarbons. European Physical Journal B, 2011, 81, 253-262.	1.5	7
16	A stripe with a local gate potential: An efficient magnetometer?. Physica Status Solidi (A) Applications and Materials Science, 2011, 208, 720-724.	1.8	0
17	Ab initioelectronic and geometrical structures of tripotassium-intercalated phenanthrene. Physical Review B, 2011, 84, .	3.2	34
18	Crystal structure and electronic states of tripotassium picene. Physical Review B, 2011, 83, .	3.2	45

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19	Fit of Pariser-Parr-Pople and Hubbard model Hamiltonians to charge and spin states of polycyclic aromatic hydrocarbons. Physical Review B, 2010, 81, .	3.2	25
20	Trapping of electrons near chemisorbed hydrogen on graphene. Physical Review B, 2010, 81, .	3.2	18
21	Hydrogen on graphene under stress: Molecular dissociation and gap opening. Physical Review B, 2010, 81, .	3.2	77
22	Magnetic molecules created by hydrogenation of polycyclic aromatic hydrocarbons. Physical Review B, 2009, 79, .	3.2	14
23	Magnetism in hydroâ€•and dehydrogenated benzene. Physica Status Solidi C: Current Topics in Solid State Physics, 2009, 6, 2139-2144.	0.8	6
24	Effects of methods and basis set on ab initio calculations of electronic transport through hydrogenated Pt nanocontacts. International Journal of Quantum Chemistry, 2008, 108, 1637-1644.	2.0	6
25	Strong covalent bonding between two graphene layers. Physical Review B, 2008, 77, .	3.2	147
26	First-principles calculation of the effect of stress on the chemical activity of graphene. Applied Physics Letters, 2008, 93, .	3.3	50
27	Transport regimes in surface disordered graphene sheets. Physical Review B, 2007, 75, .	3.2	46
28	Thermodynamic properties and electrical conductivity of a tight-binding hard-sphere model for liquid metals. Journal of Non-Crystalline Solids, 2007, 353, 3523-3527.	3.1	1
29	Hubbard Hamiltonian for the hydrogen molecule. Physical Review B, 2007, 75, .	3.2	21
30	The single-particle spectral function of quasi-one-dimensional insulating materials. Journal of Physics and Chemistry of Solids, 2006, 67, 72-76.	4.0	0
31	Quasiperiodic states in linear surface wave experiments. Philosophical Magazine, 2006, 86, 1065-1073.	1.6	5
32	Quasicrystalline and Rational Approximant Wave Patterns in Hydrodynamic and Quantum Nested Wells. Physical Review Letters, 2006, 97, 124501.	7.8	3
33	Phase transitions due to the formation of polarons in colossal magnetoresistive manganites: Monte Carlo simulations. Physical Review B, 2006, 74, .	3.2	2
34	Molecular Electronics with Gaussian98/03. Computational Chemistry - Reviews of Current Trends, 2005, , 1-46.	0.4	7
35	Topology-induced many body effects in hydrogenated Pt nanocontacts. Physical Review B, 2005, 71, .	3.2	13
36	Electrical conductivity of a tight-binding hard-sphere model for hot fluid metals. Physical Review B, 2005, 71, .	3.2	2

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37	Electronic transport and vibrational modes in a small molecular bridge:H2in Pt nanocontacts. Physical Review B, 2004, 69, .	3.2	48
38	Classical trajectories in quantum transport at the band center of bipartite lattices with or without vacancies. Physical Review B, 2004, 69, .	3.2	3
39	Conductance fluctuations in metallic nanocontacts. Physical Review B, 2004, 70, .	3.2	1
40	Density functional theory study of the interaction of monomeric water with the Ag{111} surface. Physical Review B, 2004, 69, .	3.2	53
41	Water Dimer Diffusion on Pd{111} Assisted by an H-Bond Donor-Acceptor Tunneling Exchange. Physical Review Letters, 2004, 92, 136104.	7.8	114
42	Analysis of Scanning Tunneling Spectroscopy Experiments from First Principles: The Test Case of C60 Adsorbed on Au(111). ChemPhysChem, 2003, 4, 388-392.	2.1	31
43	First-Principles Phase-Coherent Transport in Metallic Nanotubes with Realistic Contacts. Physical Review Letters, 2003, 90, 106801.	7.8	159
44	Implementing the Keldysh formalism intoab initiomethods for the calculation of quantum transport: Application to metallic nanocontacts. Physical Review B, 2003, 67, .	3.2	76
45	First-principles approach to electrical transport in atomic-scale nanostructures. Physical Review B, 2002, 66, .	3.2	186
46	Lattice-Spin Mechanism in Colossal Magnetoresistive Manganites. Physical Review Letters, 2002, 88, 136401.	7.8	64
47	Resistivity of Mixed-Phase Manganites. Physical Review Letters, 2001, 86, 135-138.	7.8	241
48	Phase separation scenario for manganese oxides. Journal of Magnetism and Magnetic Materials, 2001, 226-230, 773-774.	2.3	9
49	Conductance scaling at the band center of wide wires with pure nondiagonal disorder. Physical Review B, 2001, 65, .	3.2	8
50	Partially filled stripes in the two-dimensional Hubbard model:â€,â€,Statics and dynamics. Physical Review B, 2001, 64, .	3.2	4