IvÃ¡n Cabria

List of Publications by Year
in descending order

64 papers	3,058 citations	270111 25 h-index	175968 55 g-index
64 all docs	64 docs citations	64 times ranked	4247 citing authors

#	Article	IF	Citations
1	Grand Canonical Monte Carlo simulations of the hydrogen storage capacities of slit-shaped pores, nanotubes and torusenes. International Journal of Hydrogen Energy, 2022, 47, 11916-11928.	3.8	7
2	Assessment of density functional approximations for <scp>N₂</scp> and <scp>CO₂</scp> physisorption on benzene and graphene. Journal of Computational Chemistry, 2022, 43, 1403-1419.	1.5	3
3	Comparison of theoretical methods of the hydrogen storage capacities of nanoporous carbons. International Journal of Hydrogen Energy, 2021, 46, 12192-12205.	3.8	9
4	Hydrogen storage capacity of Li-decorated borophene and pristine graphene slit pores: A combined ab initio and quantum-thermodynamic study. Applied Surface Science, 2021, 562, 150019.	3.1	15
5	Simulations of volumetric hydrogen storage capacities of nanoporous carbons: Effect of dispersion interactions as a function of pressure, temperature and pore width. International Journal of Hydrogen Energy, 2020, 45, 5697-5709.	3.8	10
6	Magnetostatic dipolar anisotropy energy and anisotropy constants in arrays of ferromagnetic nanowires as a function of their radius and interwall distance. Journal of Physics Communications, 2020, 4, 035015.	0.5	7
7	Magnetostatic dipolar energy of large periodic Ni fcc nanowires, slabs and spheres. Applied Surface Science, 2019, 490, 352-364.	3.1	1
8	DFT simulation of hydrogen storage on manganese phosphorous trisulphide (MnPS3). International Journal of Hydrogen Energy, 2018, 43, 5903-5912.	3.8	11
9	Potential- K- Means for Load Balancing and Cost Minimization in Mobile Recycling Network. IEEE Systems Journal, 2017, 11, 242-249.	2.9	10
10	Searching for DFT-based methods that include dispersion interactions to calculate the physisorption of H2 on benzene and graphene. Journal of Chemical Physics, 2017, 146, 214104.	1.2	30
11	MRI segmentation fusion for brain tumor detection. Information Fusion, 2017, 36, 1-9.	11.7	79
12	The Storage of Hydrogen in Nanoporous Carbons. Journal of the Mexican Chemical Society, 2017, 56, .	0.2	2
13	Computing force field-based directional maps in subquadratic time. Knowledge-Based Systems, 2016, 95, 58-70.	4.0	1
14	Interaction of hydrogen with palladium clusters deposited on graphene. AIP Conference Proceedings, 2015, , .	0.3	0
15	Automated segmentation of brain tumors in MRI using potential field clustering. , 2015, , .		4
16	Automated Localization of Brain Tumors in MRI Using Potential-K-Means Clustering Algorithm. , 2015, , .		8
17	Competition between molecular and dissociative adsorption of hydrogen on palladium clusters deposited on defective graphene. RSC Advances, 2015, 5, 47945-47953.	1.7	45
18	From graphene oxide to pristine graphene: revealing the inner workings of the full structural restoration. Nanoscale, 2015, 7, 2374-2390.	2.8	95

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19	Palladium Clusters Anchored on Graphene Vacancies and Their Effect on the Reversible Adsorption of Hydrogen. Journal of Physical Chemistry C, 2014, 118, 5081-5090.	1.5	73
20	Simulation of hydrogen storage in porous carbons. Journal of Materials Research, 2013, 28, 589-604.	1.2	31
21	Evolution of the atomic structure and the magnetism of small oxygen clusters. Computational and Theoretical Chemistry, 2013, 1021, 215-221.	1.1	3
22	Adsorption and dissociation of molecular hydrogen on the edges of graphene nanoribbons. Journal of Nanoparticle Research, 2012, 14, 1.	0.8	15
23	A Mean Shift-Based Initialization Method for K-means. , 2012, , .		7
24	Density functional study of low-lying isomers of SiO4, GeO4 and CO4, and their relation to tetrahedral solid phases. European Physical Journal D, 2012, 66, 1.	0.6	0
25	Adsorption and Dissociation of Molecular Hydrogen on Palladium Clusters Supported on Graphene. Journal of Physical Chemistry C, 2012, 116, 21179-21189.	1.5	104
26	Simulated porosity and electronic structure of nanoporous carbons. Journal of Chemical Physics, 2011, 135, 104706.	1.2	37
27	Simulation of the hydrogen storage in nanoporous carbons with different pore shapes. International Journal of Hydrogen Energy, 2011, 36, 10748-10759.	3.8	65
28	Theoretical study of the transition from planar to three-dimensional structures of palladium clusters supported on graphene. Physical Review B, 2010, 81, .	1.1	122
29	Hydrogen and Hydrogen Clusters Across Disciplines. Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems, 2010, , 299-342.	0.6	0
30	Adsorption of Lithium on Finite Graphitic Clusters. Journal of Physical Chemistry C, 2009, 113, 939-941.	1.5	34
31	A Combined Experimental and Theoretical Investigation of Atomic-Scale Defects Produced on Graphite Surfaces by Dielectric Barrier Discharge Plasma Treatment. Journal of Physical Chemistry C, 2009, 113, 18719-18729.	1.5	12
32	Hydrogen storage capacities of nanoporous carbon calculated by density functional and MÃ¸ller-Plesset methods. Physical Review B, 2008, 78, .	1.1	49
33	Interaction of narrow carbon nanotubes with nitronium tetrafluoroborate salts. Journal of Chemical Physics, 2008, 128, 214703.	1.2	6
34	Shape of the hydrogen adsorption regions of MOF-5 and its impact on the hydrogen storage capacity. Physical Review B, 2008, 78, .	1.1	13
35	Hydrogen storage in pure and Li-doped carbon nanopores: Combined effects of concavity and doping. Journal of Chemical Physics, 2008, 128, 144704.	1.2	53
36	The optimum average nanopore size for hydrogen storage in carbon nanoporous materials. Carbon, 2007, 45, 2649-2658.	5.4	168

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37	Density functional calculations of hydrogen adsorption on boron nanotubes and boron sheets. Nanotechnology, 2006, 17, 778-785.	1.3	83
38	Magnetic properties of Co- and FePt-clusters. Computational Materials Science, 2006, 35, 279-282.	1.4	17
39	Density functional study of molecular hydrogen coverage on carbon nanotubes. Computational Materials Science, 2006, 35, 238-242.	1.4	54
40	Buckling in boron sheets and nanotubes. Physica Status Solidi (A) Applications and Materials Science, 2006, 203, 1105-1110.	0.8	22
41	Electrostrictive deformations in small carbon clusters, hydrocarbon molecules, and carbon nanotubes. Physical Review A, 2006, 74, .	1.0	5
42	Structural and thermal stability of narrow and short carbon nanotubes and nanostrips. Carbon, 2005, 43, 1371-1377.	5.4	38
43	Adsorption of hydrogen on normal and pentaheptite single wall carbon nanotubes. European Physical Journal D, 2005, 34, 279-282.	0.6	25
44	Electronic and magnetic properties of free and supported transition metal clusters. Phase Transitions, 2005, 78, 71-83.	0.6	3
45	Improvement of the Koradi parallel algorithm for molecular dynamics and application to the economic organization and optimization of recycling costs of waste electrical and electronic equipment. Europhysics Letters, 2005, 71, 845-851.	0.7	5
46	BeB2nanostructures: A density functional study. Physical Review B, 2005, 72, .	1.1	6
47	Enhancement of hydrogen physisorption on graphene and carbon nanotubes by Li doping. Journal of Chemical Physics, 2005, 123, 204721.	1.2	247
48	Stability and electronic structure of phosphorus nanotubes. Europhysics Letters, 2004, 65, 82-88.	0.7	52
49	Giant Magnetic Anisotropy of Single Cobalt Atoms and Nanoparticles. Science, 2003, 300, 1130-1133.	6.0	967
50	Stability of narrow zigzag carbon nanotubes. International Journal of Quantum Chemistry, 2003, 91, 51-56.	1.0	27
51	Metallic and semiconducting narrow carbon nanotubes. Physical Review B, 2003, 67, .	1.1	139
52	Largest Band Gap of All Single Walled Carbon Nanotubes. Materials Research Society Symposia Proceedings, 2003, 772, 531.	0.1	2
53	Orbital magnetism of transition-metal adatoms and clusters on the Ag and Au(001) surfaces. Physical Review B, 2002, 65, .	1.1	64
54	Electronic and Magnetic Properties of Ferromagnet-Semiconductor Heterostructure Systems. Phase Transitions, 2002, 75, 113-123.	0.6	5

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55	Magnetization profile and magnetocrystalline anisotropy of ferromagnet-semiconductor heterostructure systems. Physical Review B, 2001, 63, .	1.1	13
56	Strongly Enhanced Orbital Moments and Anisotropies of Adatoms on the Ag(001) Surface. Physical Review Letters, 2001, 86, 2146-2149.	2.9	97
57	Relativistic theory for the nuclear spin-lattice relaxation rate in ferromagnetic metals with application to5dimpurities in bcc Fe. Physical Review B, 2000, 62, 14287-14296.	1.1	4
58	Neutral atoms in ionic lattices:â€ƒStability and ground-state properties ofKCl:Ag0. Physical Review B, 2000, 62, 13356-13365.	1.1	12
59	Microscopic origin of the magnetocrystalline anisotropy energy of ferromagnetic-semiconductor multilayers. Europhysics Letters, 2000, 51, 209-215.	0.7	9
60	Optical properties of Ti2+centres in alkali halides: Theoretical investigation. Radiation Effects and Defects in Solids, 1999, 151, 281-284.	0.4	0
61	Optical properties of hole centres in alkali halides: I. Investigation with optical detection of paramagnetic resonance. Journal of Physics Condensed Matter, 1998, 10, 6473-6479.	0.7	12
62	Optical properties of hole centres in alkali halides: II. MS-X calculations. Journal of Physics Condensed Matter, 1998, 10, 6481-6490.	0.7	13
63	Stability of Silver Atoms in Chlorides: An Insight into Optical and EPR Properties. Materials Science Forum, 1997, 239-241, 171-174.	0.3	1
64	Neutral atoms in ionic lattices: Study of KCl:Ag0. International Journal of Quantum Chemistry, 1997, 61, 627-634.	1.0	7