Matic LozinÅ¡ek

List of Publications by Year
in descending order

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Version: 2024-02-01

53	22,025	236612	168136
papers	citations	25 h-index	53 g-index

58	58	58	23789
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. Journal of Physics Condensed Matter, 2009, 21, 395502.	0.7	18,183
2	XCrySDenâ€”a new program for displaying crystalline structures and electron densities. Journal of Molecular Graphics and Modelling, 1999, 17, 176-179.	1.3	1,315
3	On the HSAB based estimate of charge transfer between adsorbates and metal surfaces. Chemical Physics, 2012, 393, 1-12.	0.9	283
4	What Determines the Inhibition Effectiveness of ATA, BTAH, and BTAOH Corrosion Inhibitors on Copper?. Journal of the American Chemical Society, 2010, 132, 16657-16668.	6.6	278
5	Is the analysis of molecular electronic structure of corrosion inhibitors sufficient to predict the trend of their inhibition performance. Electrochimica Acta, 2010, 56, 745-755.	2.6	258
6	DFT Study of Interaction of Azoles with Cu(111) and Al(111) Surfaces: Role of Azole Nitrogen Atoms and Dipoleâ€“Dipole Interactions. Journal of Physical Chemistry C, 2011, 115, 24189-24197.	1.5	159
7	Fluorinated Reduced Graphene Oxide as an Interlayer in Liâ€“S Batteries. Chemistry of Materials, 2015, 27, 7070-7081.	3.2	124
8	The roles of mercapto, benzene, and methyl groups in the corrosion inhibition of imidazoles on copper: II. Inhibitorâ€“copper bonding. Corrosion Science, 2015, 98, 457-470.	3.0	109
9	Ab initio modeling of the bonding of benzotriazole corrosion inhibitor to reduced and oxidized copper surfaces. Faraday Discussions, 2015, 180, 415-438.	1.6	106
10	The relation between adsorption bonding and corrosion inhibition of azole molecules on copper. Corrosion Science, 2013, 73, 7-17.	3.0	90
11	Formation and structure of inhibitive molecular film of imidazole on iron surface. Corrosion Science, 2013, 68, 195-203.	3.0	87
12	Simplistic correlations between molecular electronic properties and inhibition efficiencies: Do they really exist?. Corrosion Science, 2021, 179, 108856.	3.0	86
13	Molecular modeling of organic corrosion inhibitors: Calculations, pitfalls, and conceptualization of moleculeâ€“surface bonding. Corrosion Science, 2021, 193, 109650.	3.0	70
14	DFT study of gas-phase adsorption of benzotriazole on Cu(111), Cu(100), Cu(110), and low coordinated defects thereon. Physical Chemistry Chemical Physics, 2011, 13, 20408.	1.3	69
15	How relevant is the adsorption bonding of imidazoles and triazoles for their corrosion inhibition of copper?. Corrosion Science, 2017, 124, 25-34.	3.0	64
16	Methane Dehydrogenation on Rh@Cu(111):Â A First-Principles Study of a Model Catalyst. Journal of the American Chemical Society, 2006, 128, 12448-12454.	6.6	60
17	Electrostatic model for treating long-range lateral interactions between polar molecules adsorbed on metal surfaces. Physical Review B, 2011, 84, .	1.1	52
18	On the consistent use of electrophilicity index and HSAB-based electron transfer and its associated change of energy parameters. Chemical Physics Letters, 2011, 507, 181-184.	1.2	52

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19	Fluorinated reduced graphene oxide as a protective layer on the metallic lithium for application in the high energy batteries. Scientific Reports, 2018, 8, 5819.	1.6	51
20	A DFT study of adsorption of imidazole, triazole, and tetrazole on oxidized copper surfaces: Cu₂O(111) and Cu₂O(111)-w/o-Cu^{CUS}. Physical Chemistry Chemical Physics, 2015, 17, 28602-28615.	1.3	45
21	Electrochemical Performance and Mechanism of Calcium Metalâ€Organic Battery. Batteries and Supercaps, 2021, 4, 214-220.	2.4	44
22	The Effect of Surface Geometry of Copper on Adsorption of Benzotriazole and Cl. Part I. Journal of Physical Chemistry C, 2014, 118, 933-943.	1.5	42
23	trans-Diastereoselective Ru(II)-Catalyzed Asymmetric Transfer Hydrogenation of Î±-Acetamido Benzocyclic Ketones via Dynamic Kinetic Resolution. Organic Letters, 2019, 21, 3644-3648.	2.4	34
24	DFT study of aqueous-phase adsorption of cysteine and penicillamine on Fe(110): Role of bond-breaking upon adsorption. Applied Surface Science, 2020, 514, 145896.	3.1	34
25	DFT Study of Azole Corrosion Inhibitors on Cu2O Model of Oxidized Copper Surfaces: I. Moleculeâ€“Surface and Clâ€“Surface Bonding. Metals, 2018, 8, 310.	1.0	30
26	Insight into the Bonding of Silanols to Oxidized Aluminum Surfaces. Journal of Physical Chemistry C, 2018, 122, 9417-9431.	1.5	25
27	Mixed Nobleâ€Gas Compounds of Krypton(II) and Xenon(VI); [F₅Xe(FKrF)AsF₆] and [F₅Xe(FKrF)₂AsF₆]. Angewandte Chemie - International Edition, 2021, 60, 8149-8156.	7.2	20
28	On the importance of time-resolved electrochemical evaluation in corrosion inhibitor-screening studies. Npj Materials Degradation, 2020, 4, .	2.6	18
29	Study Of Mercaptobenzimidazoles As Inhibitors For Copper Corrosion: Down to the Molecular Scale. Journal of the Electrochemical Society, 2021, 168, 051504.	1.3	18
30	Coordination of KrF₂ to a Naked Metal Cation, Mg²⁺. Angewandte Chemie - International Edition, 2017, 56, 6251-6254.	7.2	16
31	How relevant are molecular electronic parameters for predicting corrosion inhibition efficiency: imidazoles as corrosion inhibitors of Cu/Zr materials in NaCl solution. Corrosion Science, 2021, 193, 109900.	3.0	16
32	Syntheses, structures and Raman spectra of Cd(BF4)(AF6) (A=Ta, Bi) compounds. Journal of Fluorine Chemistry, 2011, 132, 767-771.	0.9	14
33	Reactivity of VOF₃ with N-Heterocyclic Carbene and Imidazolium Fluoride: Analysis of Ligandâ€“VOF₃ Bonding with Evidence of a Minute Ï€ Back-Donation of Fluoride. Inorganic Chemistry, 2018, 57, 13866-13879.	1.9	14
34	DFT Study of Azole Corrosion Inhibitors on Cu2O Model of Oxidized Copper Surfaces: II. Lateral Interactions and Thermodynamic Stability. Metals, 2018, 8, 311.	1.0	14
35	Latent Porosity in Alkali-Metal M2B12F12 Salts: Structures and Rapid Room-Temperature Hydration/Dehydration Cycles. Inorganic Chemistry, 2017, 56, 12023-12041.	1.9	13
36	New insights into adsorption bonding of imidazole: A viable C2â€“H bond cleavage on copper surfaces. Applied Surface Science, 2019, 479, 463-468.	3.1	13

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37	How adsorbed H, O, OH, and Cl affect plain adsorption of imidazole on copper. Corrosion Science, 2022, 205, 110443.	3.0	13
38	HF molecules and poly(hydrogen fluoride) anions as ligands to metal centers. Journal of Fluorine Chemistry, 2009, 130, 1093-1098.	0.9	12
39	Corrosion resistance of crystalline and amorphous CuZr alloys in NaCl aqueous environment and effect of corrosion inhibitors. Journal of Alloys and Compounds, 2021, 879, 160464.	2.8	12
40	Catalytic Stereoconvergent Synthesis of Homochiral Î²-CF₃, Î²-SCF₃, and Î²-OCF₃ Benzylic Alcohols. ACS Organic & Inorganic Au, 2022, 2, 396-404.	1.9	12
41	Manifestations of Weak Oâ€“HÂ·Â·Â·F Hydrogen Bonding in M(H₂O)_n(B₁₂F₁₂) Salt Hydrates: Unusually Sharp Fourier Transform Infrared Î½(OH) Bands and Latent Porosity (M = Mgâ€“Ba, Co, Ni, Zn). Inorganic Chemistry, 2018, 57, 14983-15000.	1.9	11
42	Syntheses, crystal structures and Raman spectra of Ba(BF4)(PF6), Ba(BF4)(AsF6) and Ba2(BF4)2(AsF6)(H3F4); the first examples of metal salts containing simultaneously tetrahedral BF4â¯ and octahedral AF6â¯ anions. Journal of Solid State Chemistry, 2009, 182, 2897-2903.	1.4	10
43	Origin of Surprising Attractive Interactions between Electronegative Oxygen Adatoms on Aluminum Surfaces. Journal of Physical Chemistry C, 2016, 120, 25915-25922.	1.5	9
44	Synthesis and Crystal Structure of Triammine Pentafluorido Tantalum(V) [TaF5(NH3)3]. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2013, 639, 2586-2588.	0.6	8
45	Coordination of KrF₂ to a Naked Metal Cation, Mg²⁺. Angewandte Chemie, 2017, 129, 6347-6350.	1.6	7
46	Towards dry and contaminant free Ca(BF4)2-based electrolytes for Ca plating. Journal of Power Sources Advances, 2020, 6, 100032.	2.6	7
47	The world of krypton revisited. Nature Chemistry, 2016, 8, 732-732.	6.6	5
48	Lead Fluoridooxidovanadates(V), Pb(V₂O₂F₈), Pb(VOF₅), and Mixed Valent Fluoridooxidovanadate(IV, V), Pb₃F(V₄O₃F₁₈). Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2012, 638, 2123-2128.	0.6	3
49	Hydroxylammonium Tetrafluoridooxidovanadate(V) â€“ (NH3OH)[VOF4]. Acta Chimica Slovenica, 2015, 62, 378-384.	0.2	3
50	Expanding the boron peroxide chemistry on BODIPY scaffold. Dyes and Pigments, 2021, 190, 109290.	2.0	3
51	Mixed Nobleâ€Gas Compounds of Krypton(II) and Xenon(VI); [F 5 Xe(FKrF)AsF 6] and [F 5 Xe(FKrF) 2 AsF 6]. Angewandte Chemie, 2021, 133, 8230-8237.	1.6	2
52	Nitrosonium tetrafluoridoborate, NOBF₄. IUCrData, 2021, 6, .	0.1	1
53	Silver(I) tetrafluoridooxidovanadate(V) - Ag[VOF4]. Acta Chimica Slovenica, 2014, 61, 542-7.	0.2	1