Anton Kokalj

List of Publications by Year in descending order

119 papers	30,680 citations	76196 40 h-index	21474 114 g-index
119 all docs	119 docs citations	119 times ranked	26380 citing authors

#	Article	IF	Citations
1	Corrosion inhibitors: physisorbed or chemisorbed?. Corrosion Science, 2022, 196, 109939.	3.0	113
2	DFT study of hydrogen bonding between metal hydroxides and organic molecules containing N, O, S, and P heteroatoms: clusters vs. surfaces. Chemical Physics, 2022, 559, 111539.	0.9	7
3	How adsorbed H, O, OH, and Cl affect plain adsorption of imidazole on copper. Corrosion Science, 2022, 205, 110443.	3.0	13
4	Simplistic correlations between molecular electronic properties and inhibition efficiencies: Do they really exist?. Corrosion Science, 2021, 179, 108856.	3.0	86
5	On the alleged importance of the molecular electron-donating ability and the HOMOâ€“LUMO gap in corrosion inhibition studies. Corrosion Science, 2021, 180, 109016.	3.0	50
6	Synergistic effect of 2-mercaptobenzimidazole and octylphosphonic acid as corrosion inhibitors for copper and aluminium â€“ An electrochemical, XPS, FTIR and DFT study. Corrosion Science, 2021, 182, 109082.	3.0	115
7	Two-dimensional oxide quasicrystal approximants with tunable electronic and magnetic properties. Nanoscale, 2021, 13, 10771-10779.	2.8	7
8	A model study on controlling dealloying corrosion attack by lateral modification of surfactant inhibitors. Npj Materials Degradation, 2021, 5, .	2.6	8
9	Study Of Mercaptobenzimidazoles As Inhibitors For Copper Corrosion: Down to the Molecular Scale. Journal of the Electrochemical Society, 2021, 168, 051504.	1.3	18
10	Molecular modeling of organic corrosion inhibitors: Calculations, pitfalls, and conceptualization of moleculeâ€“surface bonding. Corrosion Science, 2021, 193, 109650.	3.0	70
11	Model Study of Penetration of Cl^{â^'} Ions from Solution into Organic Self-Assembled-Monolayer on Metal Substrate: Trends and Modeling Aspects. Journal of the Electrochemical Society, 2021, 168, 071508.	1.3	7
12	The Effects of Perfluoroalkyl and Alkyl Backbone Chains, Spacers, and Anchor Groups on the Performance of Organic Compounds as Corrosion Inhibitors for Aluminum Investigated Using an Integrative Experimental-Modeling Approach. Journal of the Electrochemical Society, 2021, 168, 071506.	1.3	8
13	Coordination of a Neutral Ligand to a Metal Center of Oxohalido Anions: Fact or Fiction?. Inorganic Chemistry, 2021, 60, 11932-11947.	1.9	1
14	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
15	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
16	New inversion boundary structure in Sb-doped ZnO predicted by DFT calculations and confirmed by experimental HRTEM. Acta Materialia, 2020, 199, 633-648.	3.8	15
17	Increasing the Oxygen-Evolution Reaction Performance of Nanotubular Titanium Oxynitride-Supported Ir Nanoparticles by a Strong Metalâ€“Support Interaction. ACS Catalysis, 2020, 10, 13688-13700.	5.5	54
18	Surprising Lateral Interactions between Negatively Charged Adatoms on Metal Surfaces. Journal of Physical Chemistry Letters, 2020, 11, 7122-7126.	2.1	9

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19	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
20	On the importance of time-resolved electrochemical evaluation in corrosion inhibitor-screening studies. Npj Materials Degradation, 2020, 4, .	2.6	18
21	DFT study of n-alkyl carboxylic acids on oxidized aluminum surfaces: From standalone molecules to self-assembled-monolayers. Applied Surface Science, 2020, 525, 146156.	3.1	30
22	Editorsâ€™ Choiceâ€”The Effect of Anchor Group and Alkyl Backbone Chain on Performance of Organic Compounds as Corrosion Inhibitors for Aluminum Investigated Using an Integrative Experimental-Modeling Approach. Journal of the Electrochemical Society, 2020, 167, 061509.	1.3	29
23	Electrochemical, Surface-Analytical, and Computational DFT Study of Alkaline Etched Aluminum Modified by Carboxylic Acids for Corrosion Protection and Hydrophobicity. Journal of the Electrochemical Society, 2019, 166, C3131-C3146.	1.3	37
24	Implausibility of bidentate bonding of the silanol headgroup to oxidized aluminum surfaces. Applied Surface Science, 2019, 492, 909-918.	3.1	19
25	The peculiar case of conformations in coordination compounds of group V pentahalides with N-heterocyclic carbene and synthesis of their imidazolium salts. Journal of Fluorine Chemistry, 2019, 227, 109373.	0.9	4
26	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
27	Insight into the Bonding of Silanols to Oxidized Aluminum Surfaces. Journal of Physical Chemistry C, 2018, 122, 9417-9431.	1.5	25
28	Corrosion Inhibition. Metals, 2018, 8, 821.	1.0	3
29	An Approach to Structure-Sensitive Desorption Dynamics. , 2018, , 31-39.		0
30	Decisive Role of Perimeter Sites in Silica-Supported Ag Nanoparticles in Selective Hydrogenation of CO₂ to Methyl Formate in the Presence of Methanol. Journal of the American Chemical Society, 2018, 140, 13884-13891.	6.6	37
31	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
32	Angle-resolved desorption and removal of surface nitrogen in deNOx. Surface Science Reports, 2018, 73, 191-212.	3.8	2
33	Molecular Modeling of Corrosion Inhibitors. , 2018, , 332-345.		12
34	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
35	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
36	N 2 emission in steady-state N 2 O + CO and NO + CO reactions on Ir(110) by means of angle-resolved desorption. Applied Surface Science, 2017, 414, 153-162.	3.1	3

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37	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
38	DFT and TPD study of the role of steps in the adsorption of CO on copper: Cu(4â€‰1â€‰0) versus Cu(1â€‰0â€‰0). Journal of Physics Condensed Matter, 2017, 29, 194001.	0.7	13
39	Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901.	0.7	4,303
40	Discrete GeF₅^{â€“} Anion Structurally Characterized with a Readily Synthesized Imidazolium Based Naked Fluoride Reagent. Inorganic Chemistry, 2017, 56, 10070-10077.	1.9	12
41	Atomically Resolved Dealloying of Structurally Ordered Pt Nanoalloy as an Oxygen Reduction Reaction Electrocatalyst. ACS Catalysis, 2016, 6, 5530-5534.	5.5	65
42	Origin of Surprising Attractive Interactions between Electronegative Oxygen Adatoms on Aluminum Surfaces. Journal of Physical Chemistry C, 2016, 120, 25915-25922.	1.5	9
43	Effect of Mercapto and Methyl Groups on the Efficiency of Imidazole and Benzimidazole-based Inhibitors of Iron Corrosion. Acta Chimica Slovenica, 2016, 63, 544-559.	0.2	10
44	The roles of mercapto, benzene and methyl groups in the corrosion inhibition of imidazoles on copper: I. Experimental characterization. Corrosion Science, 2015, 98, 107-118.	3.0	90
45	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
46	Corrosion scales and passive films: general discussion. Faraday Discussions, 2015, 180, 205-232.	1.6	7
47	N2 Emission via Intermediate N2O in a Steady-State NO + CO + D2 Reaction on Stepped Pd(211) by Angle-Resolved Desorption. Journal of Physical Chemistry C, 2015, 119, 11699-11713.	1.5	8
48	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
49	Corrosion control: general discussion. Faraday Discussions, 2015, 180, 543-576.	1.6	12
50	Density Functional Theory Study of Adsorption of Benzotriazole on Cu₂O Surfaces. Journal of Physical Chemistry C, 2015, 119, 11625-11635.	1.5	42
51	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
52	Adsorption of C₂H₄ on Stepped Cu(410) Surface: A Combined TPD, FTIR, and DFT Study. Journal of Physical Chemistry C, 2014, 118, 27436-27448.	1.5	22
53	Comment on the A.B. Rochaâ€™s reply to second comment on the paper â€œOn the nature of inhibition performance of imidazole on iron surfaceâ€. Corrosion Science, 2014, 79, 215-220.	3.0	5
54	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

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55	The Effect of Surface Geometry of Copper on Dehydrogenation of Benzotriazole. Part II. Journal of Physical Chemistry C, 2014, 118, 944-954.	1.5	36
56	Molecular modeling of organic corrosion inhibitors: why bare metal cations are not appropriate models of oxidized metal surfaces and solvated metal cations. Acta Chimica Slovenica, 2014, 61, 340-9.	0.2	8
57	Formation and structure of inhibitive molecular film of imidazole on iron surface. Corrosion Science, 2013, 68, 195-203.	3.0	87
58	Comments on the â€œReply to comments on the paper â€˜On the nature of inhibition performance of imidazole on iron surfaceâ€™â€•by J.O. Mendes and A.B. Rocha. Corrosion Science, 2013, 70, 294-297.	3.0	41
59	Comments on the paper â€œOn the nature of inhibition performance of imidazole on iron surfaceâ€•by J.O. Mendes, E.C. da Silva, A.B. Rocha. Corrosion Science, 2013, 68, 286-289.	3.0	7
60	The relation between adsorption bonding and corrosion inhibition of azole molecules on copper. Corrosion Science, 2013, 73, 7-17.	3.0	90
61	An Experimental Approach to Transition States of Surface Reactions; Energy Partitioning in Repulsive Desorption. E-Journal of Surface Science and Nanotechnology, 2013, 11, 65-71.	0.1	5
62	Computer-Aided Design of the Reaction Site in Heterogeneous Catalysis. , 2013, , 1-41.		0
63	Response properties of AgCl and AgBr under an external static electric field: A density functional study. Solid State Sciences, 2012, 14, 1412-1418.	1.5	6
64	N2 emission-channel change in NO reduction over stepped Pd(211) by angle-resolved desorption. Surface Science, 2012, 606, 1029-1036.	0.8	6
65	Chemistry of the interaction between azole type corrosion inhibitor molecules and metal surfaces. Materials Chemistry and Physics, 2012, 137, 331-339.	2.0	123
66	On the HSAB based estimate of charge transfer between adsorbates and metal surfaces. Chemical Physics, 2012, 393, 1-12.	0.9	283
67	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
68	Electrostatic model for treating long-range lateral interactions between polar molecules adsorbed on metal surfaces. Physical Review B, 2011, 84, .	1.1	52
69	B3LYP investigation of response properties of alkali halides on external static electric fields. Computational Materials Science, 2011, 50, 2628-2635.	1.4	6
70	Analysis of molecular electronic structure of imidazole- and benzimidazole-based inhibitors: A simple recipe for qualitative estimation of chemical hardness. Corrosion Science, 2011, 53, 909-921.	3.0	252
71	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
72	Triazole, Benzotriazole, and Naphthotriazole as Copper Corrosion Inhibitors: I. Molecular Electronic and Adsorption Properties. ChemPhysChem, 2011, 12, 3547-3555.	1.0	53

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73	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
74	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
75	Determination of the Cu[sub 2]O Thickness on BTAH-Inhibited Copper by Reconstruction of Auger Electron Spectra. Journal of the Electrochemical Society, 2010, 157, C295.	1.3	36
76	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
77	DFT Calculations of Adsorption and Decomposition of N₂O on Rh(100). Journal of Physical Chemistry C, 2010, 114, 21444-21449.	1.5	21
78	Density Functional Theory Study of ATA, BTAH, and BTAOH as Copper Corrosion Inhibitors: Adsorption onto Cu(111) from Gas Phase. Langmuir, 2010, 26, 14582-14593.	1.6	126
79	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
80	Adsorption of Chlorine on Cu(111): A Density-Functional Theory Study. Journal of Physical Chemistry C, 2009, 113, 14363-14376.	1.5	91
81	Ethene stabilization on Cu(111) by surface roughness. Journal of Chemical Physics, 2009, 131, 024701.	1.2	17
82	Computer-Aided Design of the Reaction Site in Heterogeneous Catalysis. , 2009, , 1307-1335.		0
83	A comparative electrochemical and quantum chemical calculation study of BTAH and BTAOH as copper corrosion inhibitors in near neutral chloride solution. Electrochimica Acta, 2008, 53, 8287-8297.	2.6	197
84	What determines the catalyst's selectivity in the ethylene epoxidation reaction. Journal of Catalysis, 2008, 254, 304-309.	3.1	67
85	Adsorption of chlorine on Ag(111): No subsurface Cl at low coverage. Physical Review B, 2008, 78, .	1.1	37
86	Activated Adsorption of Ethylene on Atomic-Oxygen-Covered Ag(100) and Ag(210):â€‰ Formation of an Oxametallacycle. Journal of Physical Chemistry C, 2008, 112, 1019-1027.	1.5	21
87	Oxygen interaction at Ag(511): from chemisorption to the initial stages of oxide formation. Journal of Physics Condensed Matter, 2008, 20, 224006.	0.7	5
88	Tuning the Stoichiometry of Surface Oxide Phases by Step Morphology:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Ag</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:mn>511</mml:mn><mml:mo) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 147 Td (stretchy="false">)</mm xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Ag</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:mn>210</mml:mn><mml:mo) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 117 Td (stretchy="false">)</mm	2.9	18
89	Beyond One-Electron Reaction in Li Cathode Materials: Â Designing Li2MnxFe1-xSiO4. Chemistry of Materials, 2007, 19, 3633-3640.	3.2	245
90	Li2MnSiO4 as a potential Li-battery cathode material. Journal of Power Sources, 2007, 174, 457-461.	4.0	186

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91	Angular distributions of desorbing N2 in thermal N2O decomposition on Rh(100). Surface Science, 2007, 601, 3996-4000.	0.8	10
92	DFT Study of a Weakly Ï€-Bonded C2H4on Oxygen-Covered Ag(100). Journal of Physical Chemistry B, 2006, 110, 367-376.	1.2	20
93	Structure and dynamics of the missing-row reconstruction on O/Cu(001) and O/Ag(001). Surface Science, 2006, 600, 5074-5079.	0.8	15
94	The collimation angle shift of desorbing product N2 in a steady-state N2O+CO reaction on Rh(110). Journal of Chemical Physics, 2006, 125, 133402.	1.2	11
95	Scanning-Tunneling Microscopy, Near-Edge X-ray-Absorption Fine Structure, and Density-Functional Theory Studies of N2O Orientation on Pd(110). Japanese Journal of Applied Physics, 2006, 45, 2290-2294.	0.8	21
96	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
97	Spatial distributions of desorbing products in steady-state NO and N2O reductions on Pd(110). Journal of Chemical Physics, 2006, 124, 144711.	1.2	14
98	On-surface and sub-surface oxygen adsorption on Ag(210): Vibrational properties. Surface Science, 2005, 587, 50-54.	0.8	12
99	Orientation of nitrous oxide on palladium(110) by STM. Chemical Physics Letters, 2005, 406, 474-478.	1.2	25
100	A density-functional theory study of the interaction of N2O with Rh(110). Journal of Chemical Physics, 2005, 122, 034708.	1.2	33
101	Inclined N2 desorption in N2O reduction by D2 and CO on Pd(110). Physical Chemistry Chemical Physics, 2005, 7, 3716.	1.3	14
102	Structure and dynamics of oxygen adsorbed on Ag(100) vicinal surfaces. Physical Review B, 2004, 69, .	1.1	32
103	Multi-directional N2 desorption in N2O decomposition on Rh(110). Surface Science, 2004, 566-568, 1076-1081.	0.8	24
104	Adsorption of ethylene on stepped Ag() surfaces. Surface Science, 2004, 566-568, 1018-1023.	0.8	16
105	On-surface and subsurface adsorption of oxygen on stepped Ag(210) and Ag(410) surfaces. Surface Science, 2004, 566-568, 1107-1111.	0.8	15
106	Engineering the Reactivity of Metal Catalysts:Â A Model Study of Methane Dehydrogenation on Rh(111). Journal of the American Chemical Society, 2004, 126, 16732-16733.	6.6	80
107	N2Desorption in the Decomposition of Adsorbed N2O on Rh(110). Journal of Physical Chemistry B, 2004, 108, 3828-3834.	1.2	34
108	Co-adsorption of ethylene and oxygen on the Ag(001) surface. Surface Science, 2003, 532-535, 191-197.	0.8	14

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109	N2O interaction with Pd(110): cluster vs. slab model. Surface Science, 2003, 532-535, 213-220.	0.8	5
110	A DFT Study of the Structures of N2O Adsorbed on the Pd(110) Surface. Journal of Physical Chemistry B, 2003, 107, 2741-2747.	1.2	58
111	Computer graphics and graphical user interfaces as tools in simulations of matter at the atomic scale. Computational Materials Science, 2003, 28, 155-168.	1.4	1,618
112	Two-directional N2 desorption in thermal dissociation of N2O on Rh(110), Ir(110), and Pd(110) at low temperatures. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2002, 20, 1592-1596.	0.9	33
113	Adsorption of ethylene on the Ag() surface. Surface Science, 2002, 507-510, 62-68.	0.8	23
114	The Interaction of Ethylene with Perfect and Defective Ag(001) Surfaces. Journal of Physical Chemistry B, 2002, 106, 9839-9846.	1.2	45
115	Orientation of N2O molecule on Pd() surface. Surface Science, 2002, 506, 196-202.	0.8	36
116	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
117	Periodic DFT Study of the Pt(111):â€‰ A p(1Ã—1) Atomic Oxygen Interaction with the Surface. Journal of Physical Chemistry B, 1999, 103, 7222-7232.	1.2	32
118	Periodic density functional theory study of Pt(111): surface features of slabs of different thicknesses. Journal of Physics Condensed Matter, 1999, 11, 7463-7480.	0.7	40
119	Interaction of oxygen with the Pt(111) surface: a cluster model study. Chemical Physics Letters, 1997, 268, 43-49.	1.2	7