Jorge J Kohanoff

List of Publications by Year
in descending order

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117	5,190	101496	91828
papers	citations	36 h-index	69 g-index

121	121	121	4993
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Catalytic Role of Metal Oxides in Gold-Based Catalysts: A First Principles Study of CO Oxidation onTiO2Supported Au. Physical Review Letters, 2003, 91, 266102.	2.9	392
2	Optical properties of porous silicon: A first-principles study. Physical Review Letters, 1992, 69, 1272-1275.	2.9	359
3	Ab Initio Molecular Dynamics Simulation of a Room Temperature Ionic Liquid. Journal of Physical Chemistry B, 2005, 109, 5895-5902.	1.2	269
4	Simulations of Ionic Liquids, Solutions, and Surfaces. Accounts of Chemical Research, 2007, 40, 1138-1145.	7.6	267
5	Ab InitioMolecular Dynamics with Excited Electrons. Physical Review Letters, 1994, 73, 2599-2602.	2.9	227
6	Ab initio simulation of charged slabs at constant chemical potential. Journal of Chemical Physics, 2001, 115, 1661-1669.	1.2	206
7	Structure and Dynamics of a Confined Ionic Liquid. Topics of Relevance to Dye-Sensitized Solar Cells. Journal of Physical Chemistry B, 2005, 109, 17922-17927.	1.2	202
8	Polarization Relaxation in an Ionic Liquid Confined between Electrified Wallsâ€. Journal of Physical Chemistry B, 2007, 111, 4877-4884.	1.2	138
9	Nonadiabatic Forces in Ion-Solid Interactions: The Initial Stages of Radiation Damage. Physical Review Letters, 2012, 108, 213201.	2.9	138
10	Ferroelectricity and Isotope Effects in Hydrogen-Bonded KDP Crystals. Physical Review Letters, 2002, 89, 187602.	2.9	127
11	Electronic Stopping Power in Gold: The Role of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>d</mml:mi></mml:math>Electrons and the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi mathvariant="bold">H</mml:mi><mml:mo>/</mml:mo><mml:mi>He</mml:mi></mml:math>Anomaly. Physical Review Letters, 2012, 108, 225504.	2.9	125
12	The puzzling stability of monatomic gold wires. Surface Science, 1999, 426, L441-L446.	0.8	120
13	Simulation of interfaces between room temperature ionic liquids and other liquids. Faraday Discussions, 2005, 129, 57.	1.6	118
14	A possible new highly stable fulleride cluster: Li12C60. Chemical Physics Letters, 1992, 198, 472-477.	1.2	102
15	First-principles study of ferroelectricity and isotope effects in H-bondedKH2PO4crystals. Physical Review B, 2005, 71, .	1.1	100
16	Solid Molecular Hydrogen: The Broken Symmetry Phase. Physical Review Letters, 1997, 78, 2783-2786.	2.9	94
17	Picosecond metrology of laser-driven proton bursts. Nature Communications, 2016, 7, 10642.	5.8	80
18	Linear Scaling DFT Calculations with Numerical Atomic Orbitals. Materials Research Society Symposia Proceedings, 2001, 677, 961.	0.1	77

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19	Excess Electron Localization in Solvated DNA Bases. Physical Review Letters, 2011, 106, 238108.	2.9	77
20	Phonon spectra from short non-thermally equilibrated molecular dynamics simulations. Computational Materials Science, 1994, 2, 221-232.	1.4	65
21	Zero-point-motion effects on the structure ofC60. Physical Review B, 1992, 46, 4371-4373.	1.1	62
22	Development of Complex Classical Force Fields through Force Matching to ab Initio Data:Â Application to a Room-Temperature Ionic Liquid. Journal of Physical Chemistry B, 2006, 110, 5697-5707.	1.2	62
23	Solvation Structure and Transport of Acidic Protons in Ionic Liquids:Â A First-principles Simulation Study. Journal of Physical Chemistry B, 2006, 110, 8798-8803.	1.2	61
24	Hybrid quantum and classical mechanical Monte Carlo simulations of the interaction of hydrogen chloride with solid water clusters. Chemical Physics Letters, 1997, 280, 280-286.	1.2	57
25	Neutral and Charged 1-Butyl-3-methylimidazolium Triflate Clusters:Â Equilibrium Concentration in the Vapor Phase and Thermal Properties of Nanometric Dropletsâ€. Journal of Physical Chemistry B, 2007, 111, 4938-4950.	1.2	57
26	Excess Electron Interactions with Solvated DNA Nucleotides: Strand Breaks Possible at Room Temperature. Journal of the American Chemical Society, 2012, 134, 9122-9125.	6.6	55
27	Ab initio molecular dynamics of C70. Intramolecular vibrations and zero-point motion effects. Chemical Physics Letters, 1994, 219, 1-7.	1.2	49
28	Understanding the Interaction between Low-Energy Electrons and DNA Nucleotides in Aqueous Solution. Journal of Physical Chemistry Letters, 2015, 6, 3091-3097.	2.1	48
29	Statistical properties of the dense hydrogen plasma: Anabinitiomolecular dynamics investigation. Physical Review E, 1996, 54, 768-781.	0.8	47
30	Clusters, Liquids, and Crystals of Dialkyimidazolium Salts. A Combined Perspective from ab Initio and Classical Computer Simulations. Accounts of Chemical Research, 2007, 40, 1156-1164.	7.6	47
31	Dipole-Quadrupole Interactions and the Nature of Phase III of Compressed Hydrogen. Physical Review Letters, 1999, 83, 4097-4100.	2.9	46
32	Competition of Charge-Density Waves and Superconductivity in Sulfur. Physical Review Letters, 2007, 99, 155505.	2.9	46
33	Molecular electrostatic properties of ions in an ionic liquid. Molecular Physics, 2006, 104, 2477-2483.	0.8	43
34	Interactions between low energy electrons and DNA: a perspective from first-principles simulations. Journal of Physics Condensed Matter, 2017, 29, 383001.	0.7	42
35	Electron-induced hydrogen loss in uracil in a water cluster environment. Journal of Chemical Physics, 2014, 140, 184313.	1.2	41
36	Dry Excess Electrons in Room-Temperature Ionic Liquids. Journal of the American Chemical Society, 2011, 133, 20186-20193.	6.6	40

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37	An ab initio path integral Monte Carlo simulation method for molecules and clusters: Application to Li4 and Li5+. Journal of Chemical Physics, 1998, 108, 8848-8858.	1.2	37
38	Electronic stopping power of H and He in Al and LiF from first principles. Nuclear Instruments & Methods in Physics Research B, 2013, 303, 59-61.	0.6	32
39	Ab InitioMolecular Dynamics of Metallic Hydrogen at High Densities. Physical Review Letters, 1995, 74, 626-629.	2.9	31
40	Insights into mechanochemical reactions at the molecular level: simulated indentations of aspirin and meloxicam crystals. Chemical Science, 2019, 10, 2924-2929.	3.7	29
41	Nature of the Conduction States in the Metallic Molecular CrystalLi(NH3)4. Physical Review Letters, 1994, 73, 3133-3136.	2.9	28
42	Dynamics of Excess Electronic Charge in Aliphatic Ionic Liquids Containing the Bis(trifluoromethylsulfonyl)amide Anion. Journal of the American Chemical Society, 2013, 135, 17528-17536.	6.6	28
43	Concertedness and solvent effects in multiple proton transfer reactions: The formic acid dimer in solution. Journal of Chemical Physics, 2000, 112, 9498-9508.	1.2	27
44	Compton scatter profiles for warm dense matter. Physical Review E, 2008, 77, 046402.	0.8	27
45	Electron-phonon thermalization in a scalable method for real-time quantum dynamics. Physical Review B, 2016, 93, .	1.1	27
46	Elasticity and mechanical instabilities of diamond at megabar stresses: Implications for diamond-anvil-cell research. Applied Physics Letters, 1999, 75, 487-488.	1.5	25
47	Relevance of Heterometallic Binding Energy for Metal Underpotential Deposition. Langmuir, 2001, 17, 2219-2227.	1.6	24
48	State of the art in composition, fabrication, characterization, and modeling methods of cement-based thermoelectric materials for low-temperature applications. Renewable and Sustainable Energy Reviews, 2021, 137, 110361.	8.2	24
49	Protection of DNA against low-energy electrons by amino acids: a first-principles molecular dynamics study. Physical Chemistry Chemical Physics, 2014, 16, 24350-24358.	1.3	23
50	Interplay between Ising and six-vertex symmetries in a model for the roughening of reconstructing surfaces. Journal of Physics A, 1990, 23, 5625-5646.	1.6	19
51	Low-temperature atomic dynamics of the Si(111)-7Ã—7. Physical Review B, 1996, 54, 2642-2653.	1.1	19
52	Cement As a Waste Form for Nuclear Fission Products: The Case of ⁹⁰Sr and Its Daughters. Environmental Science & Technology, 2015, 49, 13676-13683.	4.6	19
53	Ab initio study of the structure, isotope effects, and vibrational properties in KDP crystals. Physical Review B, 2018, 98, .	1.1	19
54	Dispersion interactions in room-temperature ionic liquids: Results from a non-empirical density functional. Journal of Chemical Physics, 2011, 135, 154505.	1.2	18

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55	Evidence of Short-Range Screening in Shock-Compressed Aluminum Plasma. Physical Review Letters, 2008, 101, 075003.	2.9	17
56	Interplay between proton ordering and ferroelectric polarization in H-bonded KDP-type crystals. Computational Materials Science, 2001, 22, 87-93.	1.4	16
57	Hollow Gold Nanoparticles Produced by Femtosecond Laser Irradiation. Journal of Physical Chemistry Letters, 2020, 11, 5108-5114.	2.1	16
58	Molecular dynamics simulation of the lattice: dynamic properties. Journal of Physics Condensed Matter, 1998, 10, 4221-4229.	0.7	15
59	Pulse method of measuring thermal diffusivity and optical absorption depth for partially transparent materials. Journal of Applied Physics, 1988, 63, 1259-1264.	1.1	14
60	Porous silicon: A silicon structure with new optical properties. Progress in Quantum Electronics, 1994, 18, 201-226.	3.5	14
61	Solvation Effects on Dissociative Electron Attachment to Thymine. Journal of Physical Chemistry B, 2019, 123, 1537-1544.	1.2	14
62	Radiation Environment and Doses on Mars at Oxia Planum and Mawrth Vallis: Support for Exploration at Sites With High Biosignature Preservation Potential. Journal of Geophysical Research E: Planets, 2021, 126, e2020JE006488.	1.5	14
63	A model for the roughening of reconstructed surfaces: finite-size study and phase diagram. Journal of Physics A, 1990, 23, L209-L215.	1.6	13
64	Production of H2 by water radiolysis in cement paste under electron irradiation: A joint experimental and theoretical study. Cement and Concrete Research, 2017, 100, 110-118.	4.6	13
65	A shell model for the H-bonded ferroelectric KH2PO4. Physica B: Condensed Matter, 2009, 404, 2736-2738.	1.3	12
66	First principles simulation of damage to solvated nucleotides due to shock waves. Journal of Chemical Physics, 2019, 150, 015101.	1.2	11
67	Effect of intrinsic defects on the thermal conductivity of PbTe from classical molecular dynamics simulations. Journal of Physics Condensed Matter, 2020, 32, 045701.	0.7	11
68	An Isothermal-Isobaric Langevin Thermostat for Simulating Nanoparticles under Pressure: Application to Au Clusters. ChemPhysChem, 2005, 6, 1848-1852.	1.0	10
69	A tight binding model for water. Journal of Chemical Physics, 2011, 134, 044130.	1.2	10
70	Water radiolysis by low-energy carbon projectiles from first-principles molecular dynamics. PLoS ONE, 2017, 12, e0171820.	1.1	10
71	THEORETICAL STUDY OF LiC₆. European Physical Journal Special Topics, 1991, 01, C5-351-C5-356.	0.2	9
72	Solvation effects on equilibria: Triazoles and N-methyl piperidinol. Physical Chemistry Chemical Physics, 2002, 4, 5281-5288.	1.3	9

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73	Organic Synthesis in the Interstellar Medium by Low-Energy Carbon Irradiation. Journal of Physical Chemistry A, 2013, 117, 9666-9672.	1.1	9
74	Molecular dynamics simulation of electron trapping in sapphire. Journal of Applied Physics, 1997, 81, 3263-3267.	1.1	8
75	The status of the low-temperature phase diagram of hydrogen at the turn of the century. , 2001, 122, 297-311.		8
76	First-principles molecular dynamics simulations of the interaction of ionic projectiles with liquid water and ice. , 2008, , .		8
77	Phonons, Instabilities and Origin of Polarization in KDP Crystals. Ferroelectrics, 2010, 401, 200-206.	0.3	8
78	Universal tight binding model for chemical reactions in solution and at surfaces. I. Organic molecules. Journal of Chemical Physics, 2014, 141, 044503.	1.2	8
79	Inelastic electron injection in a water chain. Scientific Reports, 2017, 7, 45410.	1.6	8
80	On the Mechanism of the Iodideâ€“Triiodide Exchange Reaction in a Solid-State Ionic Liquid. Journal of Physical Chemistry B, 2017, 121, 6436-6441.	1.2	8
81	Effect of quantization of vibrations on the structural properties of crystals. Physical Review B, 2008, 78, .	1.1	7
82	General local and rectilinear vibrational coordinates consistent with Eckartâ€™s conditions. Physical Review A, 2009, 79, .	1.0	7
83	On the role of magnesium in a LiF:Mg,Ti thermoluminescent dosimeter. Journal of Physics Condensed Matter, 2019, 31, 025502.	0.7	7
84	Efficient ab initio calculation of electronic stopping in disordered systems via geometry pre-sampling: Application to liquid water. Journal of Chemical Physics, 2020, 153, 034113.	1.2	7
85	Characterization and Performance Enhancement of Cement-Based Thermoelectric Materials. Polymers, 2022, 14, 2311.	2.0	7
86	Determining the electronic structure and chemical potentials of molecules in solution. Physical Chemistry Chemical Physics, 2002, 4, 3016-3021.	1.3	6
87	Electronic heat transport versus atomic heating in irradiated short metallic nanowires. Physical Review B, 2019, 100, .	1.1	6
88	Effective Li-Li interactions in K1-xLixTaO3. Journal of Physics Condensed Matter, 1994, 6, 4297-4306.	0.7	5
89	Low-temperature phase in LixK1-xTaO3. Ferroelectrics, 1994, 157, 335-340.	0.3	5
90	On the Relevance of Tunneling for the Isotope Effect in KDP. Ferroelectrics, 2002, 268, 239-244.	0.3	5

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91	Ab-Initio Investigations of Pressure Effects on the Ferroelectric Instabilities in KDP and DKDP. Ferroelectrics, 2004, 301, 61-64.	0.3	5
92	Self-consistent geometry in the computation of the vibrational spectra of molecules. Physical Review A, 2009, 80, .	1.0	5
93	Universal tight binding model for chemical reactions in solution and at surfaces. II. Water. Journal of Chemical Physics, 2014, 141, 044504.	1.2	5
94	Irradiation of Water Ice by C⁺ Ions in the Cosmic Environment. Journal of Physical Chemistry A, 2014, 118, 6991-6998.	1.1	5
95	Mechanisms of Iodideâ€“Triiodide Exchange Reactions in Ionic Liquids: A Reactive Molecular-Dynamics Exploration. International Journal of Molecular Sciences, 2019, 20, 1123.	1.8	5
96	Optimal basis set for electronic structure calculations in periodic systems. Physical Review B, 2000, 62, 15499-15504.	1.1	4
97	Multiple proton translocation in biomolecular systems: concerted to stepwise transition in a simple model. Molecular Physics, 2004, 102, 1007-1014.	0.8	4
98	Universal tight binding model for chemical reactions in solution and at surfaces. III. Stoichiometric and reduced surfaces of titania and the adsorption of water. Journal of Chemical Physics, 2014, 141, 044505.	1.2	4
99	On the Quantum Description of Irradiation Dynamics in Systems of Biological Relevance. , 2017, , 277-309.		4
100	Inelastic scattering of electrons in water from first principles: cross sections and inelastic mean free path for use in Monte Carlo track-structure simulations of biological damage. Royal Society Open Science, 2022, 9, .	1.1	4
101	Shell Model Study of Local and Global Energy Barriers in KDP. Ferroelectrics, 2010, 401, 103-109.	0.3	3
102	Ab Initio Studies of H-Bonded Systems: The Cases of Ferroelectric KH2PO4 and Antiferroelectric NH4H2PO4. , 0, , .		3
103	An excitonic model for the electronâ€“hole plasma relaxation in proton-irradiated insulators. European Physical Journal D, 2021, 75, 1.	0.6	3
104	MeV irradiation of tungsten nanowires: structural modifications. Materials Research Express, 2020, 7, 055015.	0.8	3
105	On the treatment of singularities of the Watson Hamiltonian for nonlinear molecules. International Journal of Quantum Chemistry, 2011, 111, 307-317.	1.0	2
106	Bragg's additivity rule and core and bond model studied by real-time TDDFT electronic stopping simulations: The case of water vapor. Radiation Physics and Chemistry, 2022, 193, 109961.	1.4	2
107	Battery-operated STM. Journal of Microscopy, 1988, 152, 675-679.	0.8	1
108	Solid molecular phases of Hydrogen via constant-pressure first-principles Molecular Dynamics. Materials Research Society Symposia Proceedings, 1997, 499, 329.	0.1	1

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109	Simple Molecular Systems at Very High Pressures: Computer simulation studies.. Review of High Pressure Science and Technology/Koatsuryoku No Kagaku To Gijutsu, 1998, 7, 172-177.	0.1	1
110	Reply to: â€œThe puzzling stability of monatomic gold wires is the result of small fluctuationsâ€• Surface Science, 2000, 463, 213.	0.8	1
111	Structure of warm dense matter via angularly resolved x-ray scatter. Plasma Physics and Controlled Fusion, 2009, 51, 124036.	0.9	1
112	Radioactive decay of $$mathrm {{}^{90}Sr}$$ in cement: a non-equilibrium first-principles investigation. European Physical Journal D, 2021, 75, 1.	0.6	1
113	Molecular dynamics simulation of defects in Î±-Al/sub 2/O/sub 3/. , 0, , .		0
114	Ferroelectric instabilities and self-consistent mechanism for the isotopic substitution in KDP. AIP Conference Proceedings, 2003, , .	0.3	0
115	Simplified approaches to the electronic problem. , 2006, , 270-310.		0
116	Nuclear Quantum Effects on the Structural Properties of Solids. AIP Conference Proceedings, 2007, , .	0.3	0
117	Thermal conductivity of porous polycrystalline PbTe. Physical Review Materials, 2021, 5, .	0.9	0