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	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
2	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
3	Characterization and Performance Enhancement of Cement-Based Thermoelectric Materials. Polymers, 2022, 14, 2311.	2.0	7
4	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
5	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
6	An excitonic model for the electronâ€“hole plasma relaxation in proton-irradiated insulators. European Physical Journal D, 2021, 75, 1.	0.6	3
7	Radioactive decay of $$mathrm {{}^{90}Sr}$$ in cement: a non-equilibrium first-principles investigation. European Physical Journal D, 2021, 75, 1.	0.6	1
8	Thermal conductivity of porous polycrystalline PbTe. Physical Review Materials, 2021, 5, .	0.9	0
9	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
10	Hollow Gold Nanoparticles Produced by Femtosecond Laser Irradiation. Journal of Physical Chemistry Letters, 2020, 11, 5108-5114.	2.1	16
11	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
12	MeV irradiation of tungsten nanowires: structural modifications. Materials Research Express, 2020, 7, 055015.	0.8	3
13	Electronic heat transport versus atomic heating in irradiated short metallic nanowires. Physical Review B, 2019, 100, .	1.1	6
14	Solvation Effects on Dissociative Electron Attachment to Thymine. Journal of Physical Chemistry B, 2019, 123, 1537-1544.	1.2	14
15	Insights into mechanochemical reactions at the molecular level: simulated indentations of aspirin and meloxicam crystals. Chemical Science, 2019, 10, 2924-2929.	3.7	29
16	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
17	On the role of magnesium in a LiF:Mg,Ti thermoluminescent dosimeter. Journal of Physics Condensed Matter, 2019, 31, 025502.	0.7	7
18	First principles simulation of damage to solvated nucleotides due to shock waves. Journal of Chemical Physics, 2019, 150, 015101.	1.2	11

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19	Ab initio study of the structure, isotope effects, and vibrational properties in KDP crystals. Physical Review B, 2018, 98, .	1.1	19
20	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
21	Inelastic electron injection in a water chain. Scientific Reports, 2017, 7, 45410.	1.6	8
22	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
23	On the Quantum Description of Irradiation Dynamics in Systems of Biological Relevance. , 2017, , 277-309.		4
24	Interactions between low energy electrons and DNA: a perspective from first-principles simulations. Journal of Physics Condensed Matter, 2017, 29, 383001.	0.7	42
25	Water radiolysis by low-energy carbon projectiles from first-principles molecular dynamics. PLoS ONE, 2017, 12, e0171820.	1.1	10
26	Picosecond metrology of laser-driven proton bursts. Nature Communications, 2016, 7, 10642.	5.8	80
27	Electron-phonon thermalization in a scalable method for real-time quantum dynamics. Physical Review B, 2016, 93, .	1.1	27
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	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
30	Universal tight binding model for chemical reactions in solution and at surfaces. II. Water. Journal of Chemical Physics, 2014, 141, 044504.	1.2	5
31	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
32	Electron-induced hydrogen loss in uracil in a water cluster environment. Journal of Chemical Physics, 2014, 140, 184313.	1.2	41
33	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
34	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
35	Irradiation of Water Ice by C⁺ Ions in the Cosmic Environment. Journal of Physical Chemistry A, 2014, 118, 6991-6998.	1.1	5
36	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

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37	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
38	Organic Synthesis in the Interstellar Medium by Low-Energy Carbon Irradiation. Journal of Physical Chemistry A, 2013, 117, 9666-9672.	1.1	9
39	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
40	Nonadiabatic Forces in Ion-Solid Interactions: The Initial Stages of Radiation Damage. Physical Review Letters, 2012, 108, 213201.	2.9	138
41	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
42	Dry Excess Electrons in Room-Temperature Ionic Liquids. Journal of the American Chemical Society, 2011, 133, 20186-20193.	6.6	40
43	Dispersion interactions in room-temperature ionic liquids: Results from a non-empirical density functional. Journal of Chemical Physics, 2011, 135, 154505.	1.2	18
44	Excess Electron Localization in Solvated DNA Bases. Physical Review Letters, 2011, 106, 238108.	2.9	77
45	On the treatment of singularities of the Watson Hamiltonian for nonlinear molecules. International Journal of Quantum Chemistry, 2011, 111, 307-317.	1.0	2
46	A tight binding model for water. Journal of Chemical Physics, 2011, 134, 044130.	1.2	10
47	Phonons, Instabilities and Origin of Polarization in KDP Crystals. Ferroelectrics, 2010, 401, 200-206.	0.3	8
48	Shell Model Study of Local and Global Energy Barriers in KDP. Ferroelectrics, 2010, 401, 103-109.	0.3	3
49	A shell model for the H-bonded ferroelectric KH2PO4. Physica B: Condensed Matter, 2009, 404, 2736-2738.	1.3	12
50	Structure of warm dense matter via angularly resolved x-ray scatter. Plasma Physics and Controlled Fusion, 2009, 51, 124036.	0.9	1
51	General local and rectilinear vibrational coordinates consistent with Eckartâ€™s conditions. Physical Review A, 2009, 79, .	1.0	7
52	Self-consistent geometry in the computation of the vibrational spectra of molecules. Physical Review A, 2009, 80, .	1.0	5
53	Evidence of Short-Range Screening in Shock-Compressed Aluminum Plasma. Physical Review Letters, 2008, 101, 075003.	2.9	17
54	First-principles molecular dynamics simulations of the interaction of ionic projectiles with liquid water and ice. , 2008, , .		8

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55	Compton scatter profiles for warm dense matter. Physical Review E, 2008, 77, 046402.	0.8	27
56	Effect of quantization of vibrations on the structural properties of crystals. Physical Review B, 2008, 78, .	1.1	7
57	Nuclear Quantum Effects on the Structural Properties of Solids. AIP Conference Proceedings, 2007, , .	0.3	0
58	Competition of Charge-Density Waves and Superconductivity in Sulfur. Physical Review Letters, 2007, 99, 155505.	2.9	46
59	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
60	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
61	Simulations of Ionic Liquids, Solutions, and Surfaces. Accounts of Chemical Research, 2007, 40, 1138-1145.	7.6	267
62	Polarization Relaxation in an Ionic Liquid Confined between Electrified Wallsâ€. Journal of Physical Chemistry B, 2007, 111, 4877-4884.	1.2	138
63	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
64	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
65	Simplified approaches to the electronic problem. , 2006, , 270-310.		0
66	Molecular electrostatic properties of ions in an ionic liquid. Molecular Physics, 2006, 104, 2477-2483.	0.8	43
67	An Isothermal-Isobaric Langevin Thermostat for Simulating Nanoparticles under Pressure: Application to Au Clusters. ChemPhysChem, 2005, 6, 1848-1852.	1.0	10
68	Simulation of interfaces between room temperature ionic liquids and other liquids. Faraday Discussions, 2005, 129, 57.	1.6	118
69	Ab Initio Molecular Dynamics Simulation of a Room Temperature Ionic Liquid. Journal of Physical Chemistry B, 2005, 109, 5895-5902.	1.2	269
70	First-principles study of ferroelectricity and isotope effects in H-bondedKH2PO4crystals. Physical Review B, 2005, 71, .	1.1	100
71	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
72	Ab-Initio Investigations of Pressure Effects on the Ferroelectric Instabilities in KDP and DKDP. Ferroelectrics, 2004, 301, 61-64.	0.3	5

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73	Multiple proton translocation in biomolecular systems: concerted to stepwise transition in a simple model. Molecular Physics, 2004, 102, 1007-1014.	0.8	4
74	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
75	Ferroelectric instabilities and self-consistent mechanism for the isotopic substitution in KDP. AIP Conference Proceedings, 2003, , .	0.3	0
76	On the Relevance of Tunneling for the Isotope Effect in KDP. Ferroelectrics, 2002, 268, 239-244.	0.3	5
77	Ferroelectricity and Isotope Effects in Hydrogen-Bonded KDP Crystals. Physical Review Letters, 2002, 89, 187602.	2.9	127
78	Solvation effects on equilibria: Triazoles and N-methyl piperidinol. Physical Chemistry Chemical Physics, 2002, 4, 5281-5288.	1.3	9
79	Determining the electronic structure and chemical potentials of molecules in solution. Physical Chemistry Chemical Physics, 2002, 4, 3016-3021.	1.3	6
80	Relevance of Heterometallic Binding Energy for Metal Underpotential Deposition. Langmuir, 2001, 17, 2219-2227.	1.6	24
81	Interplay between proton ordering and ferroelectric polarization in H-bonded KDP-type crystals. Computational Materials Science, 2001, 22, 87-93.	1.4	16
82	Linear Scaling DFT Calculations with Numerical Atomic Orbitals. Materials Research Society Symposia Proceedings, 2001, 677, 961.	0.1	77
83	The status of the low-temperature phase diagram of hydrogen at the turn of the century. , 2001, 122, 297-311.		8
84	Ab initio simulation of charged slabs at constant chemical potential. Journal of Chemical Physics, 2001, 115, 1661-1669.	1.2	206
85	Optimal basis set for electronic structure calculations in periodic systems. Physical Review B, 2000, 62, 15499-15504.	1.1	4
86	Reply to: â€œThe puzzling stability of monatomic gold wires is the result of small fluctuationsâ€• Surface Science, 2000, 463, 213.	0.8	1
87	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
88	Dipole-Quadrupole Interactions and the Nature of Phase III of Compressed Hydrogen. Physical Review Letters, 1999, 83, 4097-4100.	2.9	46
89	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
90	The puzzling stability of monatomic gold wires. Surface Science, 1999, 426, L441-L446.	0.8	120

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91	Molecular dynamics simulation of the lattice: dynamic properties. Journal of Physics Condensed Matter, 1998, 10, 4221-4229.	0.7	15
92	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
93	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
94	Molecular dynamics simulation of electron trapping in sapphire. Journal of Applied Physics, 1997, 81, 3263-3267.	1.1	8
95	Solid Molecular Hydrogen: The Broken Symmetry Phase. Physical Review Letters, 1997, 78, 2783-2786.	2.9	94
96	Solid molecular phases of Hydrogen via constant-pressure first-principles Molecular Dynamics. Materials Research Society Symposia Proceedings, 1997, 499, 329.	0.1	1
97	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
98	Low-temperature atomic dynamics of the Si(111)-7Ã—7. Physical Review B, 1996, 54, 2642-2653.	1.1	19
99	Statistical properties of the dense hydrogen plasma: Anabinitiomolecular dynamics investigation. Physical Review E, 1996, 54, 768-781.	0.8	47
100	Ab InitioMolecular Dynamics of Metallic Hydrogen at High Densities. Physical Review Letters, 1995, 74, 626-629.	2.9	31
101	Effective Li-Li interactions in K1-xLixTaO3. Journal of Physics Condensed Matter, 1994, 6, 4297-4306.	0.7	5
102	Nature of the Conduction States in the Metallic Molecular CrystalLi(NH3)4. Physical Review Letters, 1994, 73, 3133-3136.	2.9	28
103	Ab initio molecular dynamics of C70. Intramolecular vibrations and zero-point motion effects. Chemical Physics Letters, 1994, 219, 1-7.	1.2	49
104	Porous silicon: A silicon structure with new optical properties. Progress in Quantum Electronics, 1994, 18, 201-226.	3.5	14
105	Ab InitioMolecular Dynamics with Excited Electrons. Physical Review Letters, 1994, 73, 2599-2602.	2.9	227
106	Phonon spectra from short non-thermally equilibrated molecular dynamics simulations. Computational Materials Science, 1994, 2, 221-232.	1.4	65
107	Low-temperature phase in LixK1-xTaO3. Ferroelectrics, 1994, 157, 335-340.	0.3	5
108	Zero-point-motion effects on the structure ofC60. Physical Review B, 1992, 46, 4371-4373.	1.1	62

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109	Optical properties of porous silicon: A first-principles study. Physical Review Letters, 1992, 69, 1272-1275.	2.9	359
110	A possible new highly stable fulleride cluster: Li12C60. Chemical Physics Letters, 1992, 198, 472-477.	1.2	102
111	THEORETICAL STUDY OF LiC₆. European Physical Journal Special Topics, 1991, 01, C5-351-C5-356.	0.2	9
112	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
113	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
114	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
115	Battery-operated STM. Journal of Microscopy, 1988, 152, 675-679.	0.8	1
116	Molecular dynamics simulation of defects in Î±-Al/sub 2/O/sub 3/. , 0, , .		0
117	Ab Initio Studies of H-Bonded Systems: The Cases of Ferroelectric KH2PO4 and Antiferroelectric NH4H2PO4. , 0, , .		3