Jean-Luc Fattebert

List of Publications by Year
in descending order

40	1,770	394286 19	395590 33
papers	citations	h-index	g-index

41	41	41	2040
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Modeling of additive manufacturing processes for metals: Challenges and opportunities. Current Opinion in Solid State and Materials Science, 2017, 21, 198-206.	5.6	299
2	Towards grid-basedO(N)density-functional theory methods: Optimized nonorthogonal orbitals and multigrid acceleration. Physical Review B, 2000, 62, 1713-1722.	1.1	220
3	Density functional theory for efficientab initio molecular dynamics simulations in solution. Journal of Computational Chemistry, 2002, 23, 662-666.	1.5	164
4	Mechanical properties, defects and electronic behavior of carbon nanotubes. Carbon, 2000, 38, 1703-1711.	5.4	162
5	First-principles molecular dynamics simulations in a continuum solvent. International Journal of Quantum Chemistry, 2003, 93, 139-147.	1.0	125
6	A unified electrostatic and cavitation model for first-principles molecular dynamics in solution. Journal of Chemical Physics, 2006, 124, 074103.	1.2	109
7	Computation of Maximally Localized Wannier Functions usingÂaÂsimultaneous diagonalization algorithm. Computer Physics Communications, 2003, 155, 1-6.	3.0	86
8	Linear scaling first-principles molecular dynamics with controlled accuracy. Computer Physics Communications, 2004, 162, 24-36.	3.0	55
9	A high-resolution computational model of the deforming human heart. Biomechanics and Modeling in Mechanobiology, 2015, 14, 829-849.	1.4	46
10	A numerical algorithm for the solution of a phase-field model of polycrystalline materials. Journal of Computational Physics, 2010, 229, 626-641.	1.9	43
11	Towards real-time simulation of cardiac electrophysiology in a human heart at high resolution. Computer Methods in Biomechanics and Biomedical Engineering, 2013, 16, 802-805.	0.9	40
12	Finite element approach for density functional theory calculations on locally-refined meshes. Journal of Computational Physics, 2007, 223, 759-773.	1.9	38
13	Finite Difference Schemes and Block Rayleigh Quotient Iteration for Electronic Structure Calculations on Composite Grids. Journal of Computational Physics, 1999, 149, 75-94.	1.9	36
14	Accurate and Scalable<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>O</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:mi>N</mml:mi><mml:mo) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 217 Td (stretchy="false">)</mml:mo></mml:math> Computations on Large Parallel Computers. Physical Review Letters, 2014, 112, 046401.	2.9	34
15	Optical Properties of Silicon Clusters in the Presence of Water:Â A First Principles Theoretical Analysis. Journal of the American Chemical Society, 2004, 126, 13827-13837.	6.6	31
16	Rapid Solidification in Bulk Ti-Nb Alloys by Single-Track Laser Melting. Jom, 2018, 70, 1589-1597.	0.9	30
17	A Wrench in the Works of Human Acetylcholinesterase: Soman Induced Conformational Changes Revealed by Molecular Dynamics Simulations. PLoS ONE, 2015, 10, e0121092.	1.1	28
18	Dynamic load balancing algorithm for molecular dynamics based on Voronoi cells domain decompositions. Computer Physics Communications, 2012, 183, 2608-2615.	3.0	27

#	Article	IF	Citations
19	Insight into SEI Growth in Li-Ion Batteries using Molecular Dynamics and Accelerated Chemical Reactions. Journal of Physical Chemistry C, 2021, 125, 18588-18596.	1.5	24
20	ExaAM: Metal additive manufacturing simulation at the fidelity of the microstructure. International Journal of High Performance Computing Applications, 2022, 36, 13-39.	2.4	20
21	Toward multiscale simulations of tailored microstructure formation in metal additive manufacturing. Materials Today, 2021, 51, 65-86.	8.3	16
22	Enabling particle applications for exascale computing platforms. International Journal of High Performance Computing Applications, 2021, 35, 572-597.	2.4	15
23	A mesoscopic digital twin that bridges length and time scales for control of additively manufactured metal microstructures. JPhys Materials, 2021, 4, 034012.	1.8	14
24	Matching time and spatial scales of rapid solidification: dynamic TEM experiments coupled to CALPHAD-informed phase-field simulations. Modelling and Simulation in Materials Science and Engineering, 2018, 26, 014002.	0.8	13
25	Modeling Dilute Solutions Using First-Principles Molecular Dynamics: Computing more than a Million Atoms with over a Million Cores. , 2016, , .		12
26	The basic matrix library (BML) for quantum chemistry. Journal of Supercomputing, 2018, 74, 6201-6219.	2.4	12
27	Stacking of oligo- and polythiophene cations in solution: Surface tension and dielectric saturation. Journal of Chemical Physics, 2006, 124, 194902.	1.2	11
28	Finite difference methods for ab initio electronic structure and quantum transport calculations of nanostructures. Handbook of Numerical Analysis, 2003, 10, 571-612.	0.9	10
29	MODELING THE BINDING OF CWAs TO AChE AND BuChE. Military Medical Science Letters (Vojenske) Tj ETQq1 1 0.784314 rgBT /Ove	0.2	10
30	An inverse iteration method using multigrid for quantum chemistry. BIT Numerical Mathematics, 1996, 36, 509-522.	1.0	9
31	Large-Scale First-Principles Molecular Dynamics Simulations with Electrostatic Embedding: Application to Acetylcholinesterase Catalysis. Journal of Chemical Theory and Computation, 2015, 11, 5688-5695.	2.3	9
32	Toward real-time modeling of human heart ventricles at cellular resolution: Simulation of drug-induced arrhythmias. , 2012, , .		6
33	A Scalable $O(N)$ Algorithm for Large-Scale Parallel First-Principles Molecular Dynamics Simulations. SIAM Journal of Scientific Computing, 2014, 36, C353-C375.	1.3	5
34	Efficient Computational Modeling of Human Ventricular Activation and Its Electrocardiographic Representation: A Sensitivity Study. Cardiovascular Engineering and Technology, 2018, 9, 447-467.	0.7	5
35	A parallel strategy for density functional theory computations on accelerated nodes. Parallel Computing, 2020, 100, 102703.	1.3	3
36	Papillary muscles contraction does not change ventricular wall mechanics. , 2015, , .		1

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37	ISOTHERMAL MOLECULAR DYNAMICS: A PRACTICAL STUDY. International Journal of Modern Physics C, 1993, 04, 539-551.	0.8	0
38	Optical Properties of Silicon Clusters in the Presence of Water: A First Principles Theoretical Analysis.. ChemInform, 2005, 36, no.	0.1	0
39	Finite Difference Methods in Electronic Structure Calculations. , 2015, , 521-527.		0
40	A robust solver for wavefunction-based density functional theory calculations*. Electronic Structure, 2022, 4, 015002.	1.0	0