# Jean-Luc Fattebert

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/3092266/publications.pdf

Version: 2024-02-01

| 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 | 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 |
| 2 | A robust solver for wavefunction-based density functional theory calculations*. Electronic Structure, 2022, 4, 015002. | 1.0 | 0 |
| 3 | 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 |
| 4 | Enabling particle applications for exascale computing platforms. International Journal of High Performance Computing Applications, 2021, 35, 572-597. | 2.4 | 15 |
| 5 | 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 |
| 6 | Toward multiscale simulations of tailored microstructure formation in metal additive manufacturing. Materials Today, 2021, 51, 65-86. | 8.3 | 16 |
| 7 | A parallel strategy for density functional theory computations on accelerated nodes. Parallel Computing, 2020, 100, 102703. | 1.3 | 3 |
| 8 | 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 |
| 9 | 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 |
| 10 | Rapid Solidification in Bulk Ti-Nb Alloys by Single-Track Laser Melting. Jom, 2018, 70, 1589-1597. | 0.9 | 30 |
| 11 | The basic matrix library (BML) for quantum chemistry. Journal of Supercomputing, 2018, 74, 6201-6219. | 2.4 | 12 |
| 12 | 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 |
| 13 | Modeling Dilute Solutions Using First-Principles Molecular Dynamics: Computing more than a Million Atoms with over a Million Cores. , 2016, , . | | 12 |
| 14 | 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 |
| 15 | Papillary muscles contraction does not change ventricular wall mechanics. , 2015, , . | | 1 |
| 16 | A high-resolution computational model of the deforming human heart. Biomechanics and Modeling in Mechanobiology, 2015, 14, 829-849. | 1.4 | 46 |
| 17 | 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 |
| 18 | Finite Difference Methods in Electronic Structure Calculations. , 2015, , 521-527. | | 0 |

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|---|---|---|---|
| 19 | 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 |
| 20 | 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 50 697 Td (stretchy="false">)</mml:m Computations on Large Parallel Computers. Physical Review Letters, 2014, 112, 046401. | 2.9 | 38 |
| 21 | 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 |
| 22 | MODELING THE BINDING OF CWAs TO AChE AND BuChE. Military Medical Science Letters (Vojenske) Tj ETQq0 0 0 rgBT /Overlock 10 Tf | 0.2 | 10 |
| 23 | Toward real-time modeling of human heart ventricles at cellular resolution: Simulation of drug-induced arrhythmias. , 2012, , . | | 6 |
| 24 | Dynamic load balancing algorithm for molecular dynamics based on Voronoi cells domain decompositions. Computer Physics Communications, 2012, 183, 2608-2615. | 3.0 | 27 |
| 25 | 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 |
| 26 | Finite element approach for density functional theory calculations on locally-refined meshes. Journal of Computational Physics, 2007, 223, 759-773. | 1.9 | 38 |
| 27 | A unified electrostatic and cavitation model for first-principles molecular dynamics in solution. Journal of Chemical Physics, 2006, 124, 074103. | 1.2 | 109 |
| 28 | Stacking of oligo- and polythiophene cations in solution: Surface tension and dielectric saturation. Journal of Chemical Physics, 2006, 124, 194902. | 1.2 | 11 |
| 29 | Optical Properties of Silicon Clusters in the Presence of Water: A First Principles Theoretical Analysis.. ChemInform, 2005, 36, no. | 0.1 | 0 |
| 30 | Linear scaling first-principles molecular dynamics with controlled accuracy. Computer Physics Communications, 2004, 162, 24-36. | 3.0 | 55 |
| 31 | 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 |
| 32 | First-principles molecular dynamics simulations in a continuum solvent. International Journal of Quantum Chemistry, 2003, 93, 139-147. | 1.0 | 125 |
| 33 | Computation of Maximally Localized Wannier Functions usingÂaÂsimultaneous diagonalization algorithm. Computer Physics Communications, 2003, 155, 1-6. | 3.0 | 86 |
| 34 | 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 |
| 35 | Density functional theory for efficientab initio molecular dynamics simulations in solution. Journal of Computational Chemistry, 2002, 23, 662-666. | 1.5 | 164 |
| 36 | Mechanical properties, defects and electronic behavior of carbon nanotubes. Carbon, 2000, 38, 1703-1711. | 5.4 | 162 |

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|---|---|---|---|
| 37 | Towards grid-basedO(N)density-functional theory methods: Optimized nonorthogonal orbitals and multigrid acceleration. Physical Review B, 2000, 62, 1713-1722. | 1.1 | 220 |
| 38 | 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 |
| 39 | An inverse iteration method using multigrid for quantum chemistry. BIT Numerical Mathematics, 1996, 36, 509-522. | 1.0 | 9 |
| 40 | ISOTHERMAL MOLECULAR DYNAMICS: A PRACTICAL STUDY. International Journal of Modern Physics C, 1993, 04, 539-551. | 0.8 | 0 |