# Louis Lagardre

## List of Publications by Year in Descending Order



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| 39 papers | 1,193 citations | 18 h-index | 34 g-index |
| 42 ext. papers | 1,503 ext. citations | 6.2 avg, IF | 4.47 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 39 | Computationally driven discovery of SARS-CoV-2 M inhibitors: from design to experimental validation.. *Chemical Science*, **2022**, 13, 3674-3687 | 9.4 | 2 |
| 38 | Stochastic Evaluation of Many-Body van der Waals Energies in Large Complex Systems.. *Journal of Chemical Theory and Computation*, **2022**, | 6.4 | 4 |
| 37 | Accurate Deep Learning-Aided Density-Free Strategy for Many-Body Dispersion-Corrected Density Functional Theory.. *Journal of Physical Chemistry Letters*, **2022**, 13, 4381-4388 | 6.4 | 1 |
| 36 | Development of the Quantum-Inspired SIBFA Many-Body Polarizable Force Field: Enabling Condensed-Phase Molecular Dynamics Simulations.. *Journal of Chemical Theory and Computation*, **2022**, | 6.4 | 4 |
| 35 | Tinker-HP: Accelerating Molecular Dynamics Simulations of Large Complex Systems with Advanced Point Dipole Polarizable Force Fields Using GPUs and Multi-GPU Systems. *Journal of Chemical Theory and Computation*, **2021**, 17, 2034-2053 | 6.4 | 11 |
| 34 | Implicit Solvents for the Polarizable Atomic Multipole AMOEBA Force Field. *Journal of Chemical Theory and Computation*, **2021**, 17, 2323-2341 | 6.4 | 5 |
| 33 | Atomistic Polarizable Embeddings: Energy, Dynamics, Spectroscopy, and Reactivity. *Accounts of Chemical Research*, **2021**, 54, 2812-2822 | 24.3 | 4 |
| 32 | High-resolution mining of the SARS-CoV-2 main protease conformational space: supercomputer-driven unsupervised adaptive sampling. *Chemical Science*, **2021**, 12, 4889-4907 | 9.4 | 17 |
| 31 | Interfacial Water Many-Body Effects Drive Structural Dynamics and Allosteric Interactions in SARS-CoV-2 Main Protease Dimerization Interface. *Journal of Physical Chemistry Letters*, **2021**, 12, 6218-6226 | 6.4 | 2 |
| 30 | Nuclear Quantum Effects in Liquid Water at Near Classical Computational Cost Using the Adaptive Quantum Thermal Bath. *Journal of Physical Chemistry Letters*, **2021**, 12, 8285-8291 | 6.4 | 7 |
| 29 | Reconciling NMR Structures of the HIV-1 Nucleocapsid Protein NCp7 Using Extensive Polarizable Force Field Free-Energy Simulations. *Journal of Chemical Theory and Computation*, **2020**, 16, 2013-2020 | 6.4 | 3 |
| 28 | Velocity jump processes: An alternative to multi-timestep methods for faster and accurate molecular dynamics simulations. *Journal of Chemical Physics*, **2020**, 153, 024101 | 3.9 | 4 |
| 27 | Molecular Dynamics Using Nonvariational Polarizable Force Fields: Theory, Periodic Boundary Conditions Implementation, and Application to the Bond Capacity Model. *Journal of Chemical Theory and Computation*, **2019**, 15, 6213-6224 | 6.4 | 7 |
| 26 | Towards large scale hybrid QM/MM dynamics of complex systems with advanced point dipole polarizable embeddings. *Chemical Science*, **2019**, 10, 7200-7211 | 9.4 | 30 |
| 25 | Massively Parallel Implementation of Steered Molecular Dynamics in Tinker-HP: Comparisons of Polarizable and Non-Polarizable Simulations of Realistic Systems. *Journal of Chemical Theory and Computation*, **2019**, 15, 3694-3709 | 6.4 | 12 |
| 24 | Pushing the Limits of Multiple-Time-Step Strategies for Polarizable Point Dipole Molecular Dynamics. *Journal of Physical Chemistry Letters*, **2019**, 10, 2593-2599 | 6.4 | 16 |
| 23 | Raising the Performance of the Tinker-HP Molecular Modeling Package [Article v1.0]. *Living Journal of Computational Molecular Science*, **2019**, 1, | 10.1 | 7 |

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| 22 | AMOEBA Polarizable Force Field Parameters of the Heme Cofactor in Its Ferrous and Ferric Forms. *Journal of Chemical Theory and Computation*, **2018**, 14, 2705-2720 | 6.4 | 4 |
| 21 | Tinker-HP: a massively parallel molecular dynamics package for multiscale simulations of large complex systems with advanced point dipole polarizable force fields. *Chemical Science*, **2018**, 9, 956-972 | 9.4 | 122 |
| 20 | A coherent derivation of the Ewald summation for arbitrary orders of multipoles: The self-terms. *Journal of Chemical Physics*, **2018**, 149, 124103 | 3.9 | 5 |
| 19 | Tinker 8: Software Tools for Molecular Design. *Journal of Chemical Theory and Computation*, **2018**, 14, 5273-5289 | 6.4 | 188 |
| 18 | Tinker-OpenMM: Absolute and relative alchemical free energies using AMOEBA on GPUs. *Journal of Computational Chemistry*, **2017**, 38, 2047-2055 | 3.5 | 70 |
| 17 | Channeling through Two Stacked Guanine Quartets of One and Two Alkali Cations in the Li, Na, K, and Rb Series. Assessment of the Accuracy of the SIBFA Anisotropic Polarizable Molecular Mechanics Potential. *Journal of Physical Chemistry B*, **2017**, 121, 3997-4014 | 3.4 | 18 |
| 16 | The truncated conjugate gradient (TCG), a non-iterative/fixed-cost strategy for computing polarization in molecular dynamics: Fast evaluation of analytical forces. *Journal of Chemical Physics*, **2017**, 147, 161724 | 3.9 | 15 |
| 15 | Hybrid QM/MM Molecular Dynamics with AMOEBA Polarizable Embedding. *Journal of Chemical Theory and Computation*, **2017**, 13, 4025-4033 | 6.4 | 61 |
| 14 | Truncated Conjugate Gradient: An Optimal Strategy for the Analytical Evaluation of the Many-Body Polarization Energy and Forces in Molecular Simulations. *Journal of Chemical Theory and Computation*, **2017**, 13, 180-190 | 6.4 | 28 |
| 13 | Towards scalable and accurate molecular dynamics using the SIBFA polarizable force field **2017**, | | 2 |
| 12 | Scalable improvement of SPME multipolar electrostatics in anisotropic polarizable molecular mechanics using a general short-range penetration correction up to quadrupoles. *Journal of Computational Chemistry*, **2016**, 37, 494-506 | 3.5 | 26 |
| 11 | A QM/MM Approach Using the AMOEBA Polarizable Embedding: From Ground State Energies to Electronic Excitations. *Journal of Chemical Theory and Computation*, **2016**, 12, 3654-61 | 6.4 | 100 |
| 10 | LICHEM: A QM/MM program for simulations with multipolar and polarizable force fields. *Journal of Computational Chemistry*, **2016**, 37, 1019-29 | 3.5 | 57 |
| 9 | Scalable evaluation of polarization energy and associated forces in polarizable molecular dynamics: II. Toward massively parallel computations using smooth particle mesh Ewald. *Journal of Chemical Theory and Computation*, **2015**, 11, 2589-99 | 6.4 | 37 |
| 8 | General Model for Treating Short-Range Electrostatic Penetration in a Molecular Mechanics Force Field. *Journal of Chemical Theory and Computation*, **2015**, 11, 2609-2618 | 6.4 | 79 |
| 7 | Achieving linear scaling in computational cost for a fully polarizable MM/continuum embedding. *Journal of Chemical Theory and Computation*, **2015**, 11, 694-704 | 6.4 | 40 |
| 6 | Polarizable molecular dynamics in a polarizable continuum solvent. *Journal of Chemical Theory and Computation*, **2015**, 11, 623-34 | 6.4 | 37 |
| 5 | Addressing the Issues of Non-isotropy and Non-additivity in the Development of Quantum Chemistry-Grounded Polarizable Molecular Mechanics. *Challenges and Advances in Computational Chemistry and Physics*, **2015**, 1-49 | 0.7 | 1 |

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| 4 | Scalable Evaluation of Polarization Energy and Associated Forces in Polarizable Molecular Dynamics: II.Towards Massively Parallel Computations using Smooth Particle Mesh Ewald. *Journal of Chemical Theory and Computation*, **2014**, 10, 1638-1651 | 6.4 | 66 |
| 3 | S/G-1: an ab initio force-field blending frozen Hermite Gaussian densities and distributed multipoles. Proof of concept and first applications to metal cations. *Journal of Physical Chemistry A*, **2014**, 118, 7598-612 | 2.8 | 22 |
| 2 | Quantum Calculations in Solution for Large to Very Large Molecules: A New Linear Scaling QM/Continuum Approach. *Journal of Physical Chemistry Letters*, **2014**, 5, 953-8 | 6.4 | 28 |
| 1 | Quantum, classical, and hybrid QM/MM calculations in solution: general implementation of the ddCOSMO linear scaling strategy. *Journal of Chemical Physics*, **2014**, 141, 184108 | 3.9 | 37 |