

Michael J Schnieders

List of Publications by Year in descending order

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Version: 2024-02-01

47
papers

3,351
citations

279798

23
h-index

265206

42
g-index

53
all docs

53
docs citations

53
times ranked

4037
citing authors

#	ARTICLE	IF	CITATIONS
1	Current Status of the AMOEBA Polarizable Force Field. <i>Journal of Physical Chemistry B</i> , 2010, 114, 2549-2564.	2.6	1,093
2	Tinker 8: Software Tools for Molecular Design. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5273-5289.	5.3	403
3	Genomic Landscape and Mutational Signatures of Deafness-Associated Genes. <i>American Journal of Human Genetics</i> , 2018, 103, 484-497.	6.2	214
4	Tinker-HP: a massively parallel molecular dynamics package for multiscale simulations of large complex systems with advanced point dipole polarizable force fields. <i>Chemical Science</i> , 2018, 9, 956-972.	7.4	190
5	Biomolecular electrostatics and solvation: a computational perspective. <i>Quarterly Reviews of Biophysics</i> , 2012, 45, 427-491.	5.7	152
6	Trypsin ligand binding free energies from explicit and implicit solvent simulations with polarizable potential. <i>Journal of Computational Chemistry</i> , 2009, 30, 1701-1711.	3.3	96
7	High-Throughput Genetic Testing for Thrombotic Microangiopathies and C3 Glomerulopathies. <i>Journal of the American Society of Nephrology: JASN</i> , 2016, 27, 1245-1253.	6.1	89
8	Assessment of protein structure refinement in CASP9. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 74-90.	2.6	87
9	Polarizable atomic multipole solutes in a Poisson-Boltzmann continuum. <i>Journal of Chemical Physics</i> , 2007, 126, 124114.	3.0	79
10	The Structure, Thermodynamics, and Solubility of Organic Crystals from Simulation with a Polarizable Force Field. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1721-1736.	5.3	77
11	Scalable Evaluation of Polarization Energy and Associated Forces in Polarizable Molecular Dynamics: I. Toward Massively Parallel Direct Space Computations. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1638-1651.	5.3	76
12	Polarizable Atomic Multipole Solute in a Generalized Kirkwood Continuum. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 2083-2097.	5.3	66
13	Assessment of the protein structure refinement category in CASP8. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 77, 66-80.	2.6	65
14	Hypomorphic mutations in <i>TRNT1</i> cause retinitis pigmentosa with erythrocytic microcytosis. <i>Human Molecular Genetics</i> , 2016, 25, 44-56.	2.9	64
15	<i>PDZD7</i> and hearing loss: More than just a modifier. <i>American Journal of Medical Genetics, Part A</i> , 2015, 167, 2957-2965.	1.2	54
16	Scalable Evaluation of Polarization Energy and Associated Forces in Polarizable Molecular Dynamics: II. Toward Massively Parallel Computations Using Smooth Particle Mesh Ewald. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2589-2599.	5.3	53
17	Polarizable atomic multipole X-ray refinement: application to peptide crystals. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2009, 65, 952-965.	2.5	49
18	Polarizable Molecular Dynamics in a Polarizable Continuum Solvent. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 623-634.	5.3	45

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19	Calculating binding free energies of host-guest systems using the AMOEBA polarizable force field. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 30261-30269.	2.8	44
20	Polarizable Atomic Multipole X-Ray Refinement: Particle Mesh Ewald Electrostatics for Macromolecular Crystals. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1141-1156.	5.3	40
21	Reintroducing Electrostatics into Macromolecular Crystallographic Refinement: Application to Neutron Crystallography and DNA Hydration. <i>Structure</i> , 2011, 19, 523-533.	3.3	36
22	Polarizable Atomic Multipole X-Ray Refinement: Hydration Geometry and Application to Macromolecules. <i>Biophysical Journal</i> , 2010, 98, 2984-2992.	0.5	29
23	Polarizable atomic multipole X-ray refinement: weighting schemes for macromolecular diffraction. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011, 67, 957-965.	2.5	24
24	Absolute Organic Crystal Thermodynamics: Growth of the Asymmetric Unit into a Crystal via Alchemy. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2781-2791.	5.3	24
25	Dead-End Elimination with a Polarizable Force Field Repacks PCNA Structures. <i>Biophysical Journal</i> , 2015, 109, 816-826.	0.5	24
26	A smooth and differentiable bulk-solvent model for macromolecular diffraction. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010, 66, 1024-1031.	2.5	19
27	Computational Insights for the Discovery of Non-ATP Competitive Inhibitors of MAP Kinases. <i>Current Pharmaceutical Design</i> , 2012, 18, 1173-1185.	1.9	19
28	Structural Insights into Hearing Loss Genetics from Polarizable Protein Repacking. <i>Biophysical Journal</i> , 2019, 117, 602-612.	0.5	12
29	Whole-genome sequencing reveals de-novo mutations associated with nonsyndromic cleft lip/palate. <i>Scientific Reports</i> , 2022, 12, .	3.3	11
30	Toward polarizable AMOEBA thermodynamics at fixed charge efficiency using a dual force field approach: application to organic crystals. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 30313-30322.	2.8	10
31	Novel Intragenic <i>PAX6</i> Deletion in a Pedigree with Aniridia, Morbid Obesity, and Diabetes. <i>Current Eye Research</i> , 2020, 45, 91-96.	1.5	10
32	Implicit Solvents for the Polarizable Atomic Multipole AMOEBA Force Field. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2323-2341.	5.3	10
33	Trypsin-ligand binding free energy calculation with AMOEBA. , 2009, 2009, 2328-31.		9
34	The Use of Variant Maps to Explore Domain-Specific Mutations of FGFR1. <i>Journal of Dental Research</i> , 2017, 96, 1339-1345.	5.2	7
35	Characterization of a TP53 Somatic Variant of Unknown Function From an Ovarian Cancer Patient Using Organoid Culture and Computational Modeling. <i>Clinical Obstetrics and Gynecology</i> , 2020, 63, 109-119.	1.1	7
36	In Silico and In Vivo Analysis of Amino Acid Substitutions That Cause Laminopathies. <i>International Journal of Molecular Sciences</i> , 2021, 22, 11226.	4.1	7

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37	Nanophthalmos patient with a THR518MET mutation in MYRF, a case report. BMC Ophthalmology, 2020, 20, 388.	1.4	5
38	LADD syndrome with glaucoma is caused by a novel gene. Molecular Vision, 2017, 23, 179-184.	1.1	5
39	Scalable Indirect Free Energy Method Applied to Divalent Cation-Metalloprotein Binding. Journal of Chemical Theory and Computation, 2019, 15, 4602-4614.	5.3	4
40	A novel mutation (LEU396ARG) in OPA1 is associated with a severe phenotype in a large dominant optic atrophy pedigree. Eye, 2018, 32, 843-845.	2.1	2
41	A SURGICAL GUIDE TO ACCURATELY PLACE PINS OR NAILS WITHIN THE FEMORAL HEAD. Journal of Musculoskeletal Research, 1999, 03, 233-237.	0.2	1
42	Biomolecular Structure Refinement & Prediction using Dead-End Elimination with a Polarizable Force Field. Biophysical Journal, 2014, 106, 407a.	0.5	1
43	X-Ray Crystallography Refinement as Ewald Intended: From Drug Design to Ribosome Crystals. Biophysical Journal, 2010, 98, 177a.	0.5	0
44	Bayesian Modeling of Crystallographic Disorder. Biophysical Journal, 2012, 102, 225a.	0.5	0
45	Pharmaceutical Applications of the Polarizable Amoeba Potential, Including Protein-Ligand Binding Affinity and Drug Solubility, using the Force Field X Software. Biophysical Journal, 2012, 102, 409a-410a.	0.5	0
46	Protein Sequence Optimization with a Polarizable Force Field: Insights from PDZ Domains. Biophysical Journal, 2016, 110, 345a-346a.	0.5	0
47	Polarizable Amoeba Force Field Metadynamics with Minimization Predicts Missing Protein Loops. Biophysical Journal, 2017, 112, 55a.	0.5	0