

# Eliot Boulanger

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/11118887/publications.pdf>

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9  
papers

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citations

1040056

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docs citations

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606  
citing authors

#	ARTICLE	IF	CITATIONS
1	Solvent Boundary Potentials for Hybrid QM/MM Computations Using Classical Drude Oscillators: A Fully Polarizable Model. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4527-4538.	5.3	114
2	Optimized Lennard-Jones Parameters for Druglike Small Molecules. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3121-3131.	5.3	44
3	QM/MM methods for free energies and photochemistry. <i>Current Opinion in Structural Biology</i> , 2018, 49, 72-76.	5.7	43
4	Toward QM/MM Simulation of Enzymatic Reactions with the Drude Oscillator Polarizable Force Field. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1795-1809.	5.3	40
5	Quantum mechanics/molecular mechanics dual Hamiltonian free energy perturbation. <i>Journal of Chemical Physics</i> , 2013, 139, 064105.	3.0	39
6	Hybrid Quantum Mechanics/Molecular Mechanics/Coarse Grained Modeling: A Triple-Resolution Approach for Biomolecular Systems. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1809-1818.	5.3	39
7	Importance of MM Polarization in QM/MM Studies of Enzymatic Reactions: Assessment of the QM/MM Drude Oscillator Model. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2954-2961.	5.3	34
8	Chemical substitutions in the selectivity filter of potassium channels do not rule out constricted-like conformations for C-type inactivation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 11145-11150.	7.1	29
9	A microiterative intrinsic reaction coordinate method for large QM/MM systems. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 14188.	2.8	10