

# **TINKER – *Software Tools for Molecular Design***

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**Washington University in Saint Louis (WU), The University of Texas at Austin  
(UT Austin), and Sorbonne Université (Sorbonne)**

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**“TINKER 8: Software Tools for Molecular Design**, Joshua A. Rackers, Zhi Wang, Chao Lu, Marie L. Laury, Louis Lagardère, Michael J. Schnieders, Jean-Philip Piquemal, Pengyu Ren and Jay W. Ponder, *Journal of Chemical Theory and Computation*, 14, 5273-5289, 2018.  
(DOI: 10.1021/acs.jctc.8b00529; PMCID: PMC6335969)”

Considering the use of the specific Tinker-HP code, included in the Tinker distribution, any published work which utilizes Tinker-HP shall give, in addition to the main Tinker reference, appropriate acknowledgement to the Tinker-HP developer community's contribution by including the following reference:

**“Tinker-HP: A Massively Parallel Molecular Dynamics Package for Multiscale Simulations of Large Complex Systems with Advanced Polarizable Force Fields**, Louis Lagardère, Luc-Henri Jolly, Filippo Lipparini, Félix Aviat, Benjamin Stamm, Zhifeng F. Jing, Matthew Harger, G. Andres Cisneros, Nohad Gresh, Yvon Maday, Pengyu Ren, Jay W. Ponder, Jean-Philip Piquemal, *Chemical Science*, 9, 956-972, 2017, DOI: 10.1039/c7sc04531j”

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**“Tinker-OpenMM: Absolute and Relative Alchemical Free Energies using AMOEBA on GPUs**. Matthew Harger, Daniel Li, Zhi Wang Kevin Dalby, Louis Lagardère, Jean-Philip Piquemal, Jay Ponder, Pengyu Ren, *Journal of Computational Chemistry*, 38, 2047-2055, 2017, DOI 10.1002/jcc.24853”

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