TINKER – Software Tools for Molecular Design Version 8.9 June 2021

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- "TINKER 8: A Modular Software Package for Molecular Design and Simulation. Joshua A. Rackers, Marie L. Laury, Chao Lu, Zhi Wang, Louis Lagardère, Jean-Philip Piquemal, Pengyu Ren, Jay W. Ponder, *Journal of Chemical Theory and Computation*, 14, 5273-5289, 2018, DOI 10.1021/acs.jctc.8b00529"

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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