

## List of Publications

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8. **Korol, R.**; Rosa-Raíces J.L., Bou-Rabee, N.; Miller III, T.F. Dimension-free path-integral molecular dynamics without preconditioning. *J. Chem. Phys.* **2020**, 152, 104102. DOI: [10.1063/1.5134810](https://doi.org/10.1063/1.5134810)
7. Elbridge, D. L.; **Korol, R.**, Lloyd, M.K.; Turner, A.C.; Webb, M.A.; Miller III, T.F.; Stolper D.A. Comparison of Experimental vs Theoretical Abundances of  $^{13}\text{CH}_3\text{D}$  and  $^{12}\text{CH}_2\text{D}_2$  for Isotopically Equilibrated Systems from 1 to 500 °C. *ACS Earth Space Chem.* **2019**, 3 (12), 2747-2764. DOI: [10.1021/acsearthspacechem.9b00244](https://doi.org/10.1021/acsearthspacechem.9b00244)
6. **Korol, R.**; Bou-Rabee, N.; Miller III, T.F. Cayley modification for strongly stable path-integral and ring-polymer molecular dynamics. *J. Chem. Phys.* **2019**, 151 (12), 124103. DOI: [10.1063/1.5120282](https://doi.org/10.1063/1.5120282)
5. **Korol R.**; Segal D. Machine Learning Prediction of DNA Charge Transport. *J. Phys. Chem. B*, **2019**, 123 (13), pp 2801 — 2811. DOI: [10.1021/acs.jpcc.8b12557](https://doi.org/10.1021/acs.jpcc.8b12557)
4. **Korol, R.**; Segal, D. From exhaustive simulations to key principles in DNA nanoelectronics. *J. Phys. Chem. C* **2018** 122 (8), 4206-4216. DOI: [10.1021/acs.jpcc.7b12744](https://doi.org/10.1021/acs.jpcc.7b12744).
3. **Korol, R.**; Kilgour, M.; Segal, D. ProbeZT: Simulation of transport coefficients of molecular electronic junctions under environmental effects using Büttiker's probes. *Comp. Phys. Comm.* **2018** 224, 396-404. DOI: [10.1016/j.cpc.2017.10.005](https://doi.org/10.1016/j.cpc.2017.10.005)
2. **Korol, R.**; Kilgour, M.; Segal, D. Thermopower Of Molecular Junctions: Tunneling To Hopping Crossover In DNA. *J. Chem. Phys.* **2016**, 145 (22), 224702. DOI: [10.1063/1.4971167](https://doi.org/10.1063/1.4971167)
1. Longobardi, L.E.; Zatsepin, P.; **Korol, R.**; Liu, L.; Grimme, S.; Stephan D.W. Reactions Of Boron-Derived Radicals With Nucleophiles. *J. Am. Chem. Soc.* **2016**, 139 (1), pp 426—435. DOI: [10.1021/jacs.6b11190](https://doi.org/10.1021/jacs.6b11190)