List of Publications

7. Elbridge, D. L.; **Korol, R.**, Lloyd, M.K.; Turner, A.C.; Webb, M.A.; Miller III, T.F. and Stolper D.A. Comparison of Experimental vs Theoretical Abundances of $^{13}CH_3D$ and $^{12}CH_2D_2$ for Isotopically Equilibrated Systems from 1 to 500 °C. *ACS Earth Space Chem.* **2019**, 3 (12), 2747-2764. DOI: 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
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.jpcb.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.
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
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
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