List of Publications

13. **Korol*, R.**; Chen, X.; Franco* I. High-frequency tails in spectral densities. *J. Phys. Chem. A* **2025**. DOI: 10.1021/acs.jpca.5c00943

12. Turner*, A.C.; **Korol, R.**; Bill, M.; Stolper, D.A. Stable isotope equilibria in dihydrogen-water-methane-ethane-propane system. Part 2: Experimental determination of hydrogen isotopic equilibrium for ethane-H2 from 30–200°C and propane-H2 from 75–200°C. *Geochim. et Cosmochim. Acta* **2025**, 396, 91-106. DOI: 10.1016/j.gca.2025.02.033

11. **Korol*, R.**; Turner, A.C.; Nandi, A.; Bowman, J.M.; Goddard III, W.A.; Stolper, D.A. Stable isotope equilibria in dihydrogen-water-methane-ethane-propane system. Part 1: Path-integral calculations with CCSD(T) quality potentials. *Geochim. et Cosmochim. Acta* **2025**, 396, 71-90. DOI: 10.1016/j.gca.2025.02.028

10. Turner, A.C.; **Korol, R.**; Elbridge, D. L.; Bill, M.; Miller III, T.F.; Stolper* D.A. Experimental and theoretical determinations of hydrogen isotopic equilibrium in the system CH4-H2-H2O from 3 to 200°C. *Geochim. et Cosmochim. Acta* **2021**, 314, 223-269. DOI: 10.1016/j.gca.2021.04.026

9. (Editors' Pick) **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

8. 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 $^{13}CH_3D$ 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

7. (Editors' Choice) 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 $^{13}CH_3D$ 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. (Editors' Pick) **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