

List of Publications

14. Tiwari, V; Korol, R; Franco*, I Robust Purely Optical Signatures of Floquet States in Laser-Dressed Crystals. *Phys. Rev. Lett.* **2025**, 135 (18), 186901. DOI: [10.1103/5ywx-7db5](https://doi.org/10.1103/5ywx-7db5)
13. Korol*, R; Chen, X; Franco*, I High-Frequency Tails in Spectral Densities. *J. Phys. Chem. A* **2025**, 129 (15), 3587-3596. DOI: [10.1021/acs.jpca.5c00943](https://doi.org/10.1021/acs.jpca.5c00943)
12. Turner*, A C; Korol, R; Bill, M; Stolper, D A Stable isotope equilibria in the dihydrogen-water-methane-ethane-propane system. Part 2: Experimental determination of hydrogen isotopic equilibrium for ethane-H₂ from 30 to 200 °C and propane-H₂ from 75 to 200 °C. *Geochim. Cosmochim. Acta* **2025**, 396, 91-106. DOI: [10.1016/j.gca.2025.02.033](https://doi.org/10.1016/j.gca.2025.02.033)
11. Korol*, R; Turner, A C; Nandi, A; Bowman, J M; Goddard, W A; Stolper, D A Stable isotope equilibria in the dihydrogen-water-methane-ethane-propane system. Part 1: Path-integral calculations with CCSD(T) quality potentials. *Geochim. Cosmochim. Acta* **2025**, 396, 71-90. DOI: [10.1016/j.gca.2025.02.028](https://doi.org/10.1016/j.gca.2025.02.028)
10. Turner, A C; Korol, R; Eldridge, D L; Bill, M; Conrad, M E; Miller, 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. Cosmochim. Acta* **2021**, 314, 223-269. DOI: [10.1016/j.gca.2021.04.026](https://doi.org/10.1016/j.gca.2021.04.026)
9. Korol, R; Rosa-Raíces, J L; Bou-Rabee, N; Miller*, T F Dimension-free path-integral molecular dynamics without preconditioning. *J. Chem. Phys.* **2020**, 152 (10), 104102. DOI: [10.1063/1.5134810](https://doi.org/10.1063/1.5134810)
8. Eldridge, D L; Korol, R; Lloyd, M K; Turner, A C; Webb, M A; Miller, T F; Stolper*, D A Comparison of Experimental vs Theoretical Abundances of ¹³CH₃D and ¹²CH₂D₂ 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)
7. Korol, R; Bou-Rabee, N; Miller*, 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)
6. Korol, R; Segal*, D Machine Learning Prediction of DNA Charge Transport. *J. Phys. Chem. B* **2019**, 123 (13), 2801-2811. DOI: [10.1021/acs.jpcc.8b12557](https://doi.org/10.1021/acs.jpcc.8b12557)
5. 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)
4. Korol, R; Kilgour, M; Segal*, D ProbeZT: Simulation of transport coefficients of molecular electronic junctions under environmental effects using Büttiker's probes. *Comput. Phys. Commun.* **2018**, 224, 396-404. DOI: [10.1016/j.cpc.2017.10.005](https://doi.org/10.1016/j.cpc.2017.10.005)
3. 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)

2. 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), 426-435. DOI: [10.1021/jacs.6b11190](https://doi.org/10.1021/jacs.6b11190)
1. Korol*, R V; Yanchuk, O M; Marchuk, O V; Orlov, V F; Moroz, I A; Vyshnevskyi, O A Size Stabilizers in Two-electrode Synthesis of ZnO Nanorods. *Phys. Chem. Solid St.* **2021**, 22 (2), 380-387. DOI: [10.15330/pcss.22.2.380-387](https://doi.org/10.15330/pcss.22.2.380-387)