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**. 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**. 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**. DOI: 10.1016/j.gca.2021.04.026
9. **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
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6. **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
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.
4. **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
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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), pp 426—435. DOI: 10.1021/jacs.6b11190
1. **Korol, R.V.**; Yanchuk O.M; Marchuk O.V. Orlov V.F; Moroz I.A. and Vyshnevskyi O.A. Size Stabilizers in Two-electrode Synthesis of *ZnO* Nanorods. *Phys.& Chem. of Solid State* **2021**, 22(2), pp 380–387. DOI: 10.15330/pcss.22.2.380-387