

P5528: UTILIZATION OF NEURAL NETWORKS FOR GPU-ACCELERATED DIFFUSION MONTE CARLO FOR VIBRATIONAL PROBLEMS

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- Diffusion Monte Carlo (DMC) is a great method to get ZPE and ground state wave functions of systems that do not follow harmonic approximation, but it's expensive due to the number of potential energy evaluations required.

- We developed a method of utilizing GPU-accelerated Neural Network to achieve the same level of accuracy but with a great reduction in computation time compared to conventional method

