Quantizing vibrational modes - surface hopping simulations and machine learning algorithms

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Advances in machine learning algorithms have found applications in non-adiabatic dynamics. Recent works have explored fitting electronic potential energy surfaces using machine learning algorithms for surface hopping simulations.[1-2] Although surface hopping simulations usually are applied to include electronic non-adiabatic effects, this method can also be applied to include quantum nuclear effects of select vibrational modes.[3] This work explores fitting vibrational energy surfaces using a machine-learning algorithm. We will show for model potential energy surfaces that machine-learning algorithms can generate accurate vibronic dynamics with very few training data points.

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