

# Physics-Informed Neural Networks for determination of Vibrational Energy Levels of the HCl Molecule

## Abstract

### Background:

Understanding vibrational energy levels in diatomic molecules is fundamental to molecular spectroscopy and quantum chemistry, as these levels govern molecular structure and dynamics. However, conventional numerical approaches often rely on predefined analytical wavefunctions or supervised datasets, which can limit their applicability in the presence of anharmonic molecular interactions.

### Purpose:

The purpose of this work is to develop a physics-informed neural network (PINN) framework to accurately compute the vibrational energy levels of the hydrogen chloride (HCl) molecule in a fully unsupervised manner.

### Methods:

The vibrational dynamics of the HCl molecule are modeled using the one-dimensional time-independent Schrödinger equation, with the interatomic interaction described by the Morse potential to account for anharmonic effects. A PINN is constructed to simultaneously learn the vibrational wavefunctions, energy eigenvalues, and optimized potential parameters. The training process minimizes a composite loss function incorporating the Schrödinger equation residual, boundary conditions, normalization, and orthogonality constraints.

### Results:

The optimized Morse potential parameters and the computed vibrational energy levels obtained from the PINNs show strong agreement with theoretical values. The network successfully captures the anharmonic vibrational behavior of the HCl molecule and accurately predicts multiple vibrational states without the use of labeled data.

### Conclusions:

Overall this work shows that Physics informed neural network (PINNs) serves as powerful method to simultaneously determine the vibrational frequencies and molecular potential parameters, establishing PINNs as a powerful and data efficient framework for molecular spectroscopy and computational quantum chemistry.

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