Contribution ID: **2** Type: **not specified**

Harnessing neural networks for simulations of rotational-vibrational dynamics of floppy molecules

This project builds upon a novel method recently developed in our group, which employs normalising flows (invertible neural networks) for solving the Schrödinger equation. This approach has demonstrated significant advancements in simulating the quantum vibrational dynamics of molecules, outperforming traditional variational methods. The current project's objective is to expand this methodology to also include the rotational dynamics of molecules, a crucial aspect in studies of floppy molecular systems. The successful candidate will work together with a PhD student and a postdoc focusing on the same or closely related topics. Applicants are expected to possess at least an intermediate level in Python programming and understanding of machine learning, specifically in the implementation and optimisation of neural networks using Python. A basic knowledge of quantum mechanics is essential.

Group

FS-CFEL-CMI

Project Category

A6. Theory and computing

Special Qualifications

Python, machine learning using Python, basic knowledge of quantum mechanics

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