Title: PREDICTING AND OPTIMIZING ORGANIC MATERIAL PROPERTIES WITH QUANTUM MACHINE LEARNING (QML) FOR EFFICIENT OLEDs DEVELOPMENT

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Abstract

Nowadays, the world's electricity consumption is heavily used for lighting and display purposes. The current technology, which is dominated by liquid crystal displays (LCD) and plasma screens, is increasingly being challenged by a new technology using light-emitting diodes (OLED) based on organic materials[1], allowing for extra-flat and flexible displays. OLEDs have the advantage of consuming little energy while developing high luminance. However, these devices are expensive and their development is long. The evaluation of the properties of organic materials is therefore necessary to accelerate the development of OLEDs. For this purpose, experimental and computational methods have been used. However, they have proven to be costly in terms of time and hardware resources. Machine learning (ML)[2], which is based on big data, has reduced the evaluation time considerably, but is still relatively time consuming for large databases. It is therefore interesting to integrate quantum algorithms[3] into ML programs (QML, Quantum machine learning)[4] to efficiently predict and optimize the properties of organic materials potentially usable to improve the efficiency of Oleds. In this work, we use Quantum Neural Networks (QNN)[[5, 6, 7]] to predict and optimize properties such as energy gap, current density, response time, Intensity-voltage-luminance (I-V-L) characteristic, and so on. A brief review of the literature will be provided, including applications and a description of how OLEDs work, as well as the methods and tools used in this project.

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