**Implementation of machine learning techniques to help optimize molecular systems in solar cells.**

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**Abstract**

Solar cells show us an interesting path towards the use of renewable energy, clean with the environment, and that helps us to mitigate the effect or footprint that we leave on the planet, therefore, efficient ways for conversion are sought of solar energy into electricity, such as the use of materials, seeking the best properties that allow the optimal conversion of energy. In this work for this purpose we use quantum chemistry techniques and programming support with artificial intelligence and machine learning models that allow us to optimize calculations and get closer to reality by calibrating results with Gaussian regression models that are developed in Python code, finally, through the Scharber model, find the PCE (power conversion efficiency) and calibrate with artificial intelligence to find the best candidate molecules to synthesize. The results show that artificial intelligence helps to decrease the RSME (root mean square error) between the real and calculated values, thus reducing the number of candidate molecules to be synthesized, the latter being an important factor due to the complexity and expense of resources that they would involve synthesizing a complete set of molecules that according to the present method would be useless to use.

***Keywords:*** Machine Learning, artificial Intelligence, Chemistry, Quantum, DFT, Scharber.