Development of a Rapidly Calculating Energy Gap (rCEG) AI Model for Instantaneous Determination of the HOMO-LUMO Gap

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The difference in energy between the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Orbital (LUMO) is known as the HOMO-LUMO Gap. It has a variety of applications in industries from drug design to organic solar cells. Such is the reason why the HOMO-LUMO Gap is employed by many researchers in these fields. However, the HOMO-LUMO Gap is computationally inefficient due to the advanced quantum mechanical calculations needed to calculate its value. To solve this problem, I developed the Rapidly Calculating Energy Gap (rCEG) AI Model. Machine learning offers the key to finding the HOMO-LUMO Gap by bypassing the inefficient conventional calculations. Thus, a streamlined Quantum Machine Learning (QML) approach is preferable. Through the Rapidly Calculating Energy Gap (rCEG) AI model, the HOMO-LUMO Gap can be predicted with a satisfying degree of certainty. The model accesses the molecule's molfile along with various descriptors of the molecule. Reciprocal Net, a digital database of molecular structures and software tools, was used as data to train and validate rCEG. The true HOMO-LUMO gap was calculated through the PSI-4 open-source library. Findings indicate rCEG had a low mean absolute error of 0.003161 with only 16 epochs. By simplifying the calculations in Molecular Orbital Theory, rCEG has the potential to facilitate innovation in the quantum chemistry field by revolutionizing how to calculate the HOMO-LUMO Gap.

Awards Won:

American Chemical Society: Second Award of $3,000