

Applications of Machine Learning in Predicting Electronic Properties in Organic Semiconductor Materials

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Predicting electronic properties like the band gaps, ionization potentials, and electron affinities is crucial for designing organic semiconductor materials. Traditionally, one common and efficient way to support this design process is by building quantitative structure-property relationship (QSPR) models. We have developed a new quantum mechanical based QSPR models called Degree of Partial π Overlap (DPO) for predicting these properties in polycyclic aromatic hydrocarbons (PAHs) and their derivatives, which are known to serve as core platform in organic semiconductor material synthesis. These DPO models are shown to achieve accurate predictions within 0.1 eV. However, a significant challenge in QSPR is to derive accurate model descriptors, which is time-consuming and resource intensive. To overcome these obstacles, we utilize machine learning (ML) techniques. The ML models in our studies optimize parameters faster, reduce data requirements, and improve generalization using simpler inputs like SMILES strings of molecular structures instead of detailed descriptors. This transition from manual optimization QSPR methods to practical ML based techniques while maintaining accuracy within an acceptable range, would advance the future of material design.

References

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