## Quantitative Structure–Property Relationship in Predicting Electronic Properties of Polycylic Aromatic Hydrocarbons and Derivatives from Degree of $\pi$-Orbital Overlap to High-Throughput Screening

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**Poster**
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In our quest to revolutionize the prediction of electronic properties in organic semiconductors, we have advanced the ability to predict key properties such as the Highest Occupied Molecular Orbital-Lowest Unoccupied Molecular Orbital (HOMO-LUMO) gap, ionization potentials, and electron affinities for polycyclic aromatic hydrocarbons (PAHs) and their derivatives. Initially, we manually developed QSPR models using the "degree of $\pi$-orbital overlap" (DPO) descriptor, achieving accurate predictions within 0.10 eV using Density Functional Theory. However, defining descriptor notation was time-consuming and resource-intensive. To enhance efficiency and precision, we transitioned to machine learning (ML) techniques. ML optimized the DPO parameters, reducing data requirements while maintaining high accuracy. Using the Weisfeiler-Lehman graph kernel method and Gaussian process regressor, our ML-enhanced models predicted electronic properties across 2131 aromatic molecules with remarkable precision, achieving root-mean-square deviations as low as 0.15 eV. This blend of DPO descriptors and ML techniques confirms the robustness of the DPO model and sets the stage for future advancements in organic semiconductors. Our journey from manual methods to sophisticated ML techniques highlights the dynamic evolution of our approach and its transformative impact on predicting electronic properties of PAH-based organic materials.

### References

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