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ABSTRACT

Although organic chromogenic materials are critical for optoelectronic displays and imaging, accurate prediction of their maximum absorption wavelength (λ_{max}) remains challenging: quantum chemical methods have long research and development cycles, and existing machine learning (ML) models lack physical constraints in limited-sample scenarios. Here, we propose an oscillator strength-driven ML framework (OS-ML), using excitation energy and transition dipole moment decomposed from oscillator strength as core physical descriptors. On a 74-molecule dataset, the optimal OS-ML-XGBoost model achieves a minimum prediction error of 0.6 nm, with an average deviation only 40% that of time-dependent density functional theory. This work provides an efficient approach for predicting the optical performance of organic optoelectronic materials in limited-sample scenarios.

Organic chromogenic materials are core functional materials with rich tunable optical properties, widely applied in optoelectronic devices, imaging, and solar energy conversion.[1–5] Precise regulation of their molecular structure is critical for color-rendering performance, which originates from electronic transitions between the ground and excited states.[1,2] The maximum absorption wavelength (λ_{max}) is a key indicator of the molecular energy gap and transition energy, directly determining material applications and serving as a core consideration in the molecular design.[6]

Accurate prediction of λ_{max} is essential for the rational molecular design, but traditional experimental trial-and-error and time-dependent density functional theory (TD-DFT) calculations face bottlenecks: experiments are time-consuming and costly, while quantum chemical methods scale exponentially with molecular size and often show large deviations from experimental results.[7,8] Developing efficient, accurate λ_{max} prediction methods has thus become a pressing research priority.

In recent years, machine learning (ML) has emerged as a powerful tool for predicting molecular optical properties, offering significant computational efficiency advantages over traditional quantum chemical methods.[9–16] While ML can learn structure–property relationships from experimental and computational data, most models rely solely on structural features, lacking explicit physical mechanism constraints, leading to insufficient accuracy and interpretability in limited-sample scenarios.[17]

Existing research has shown that integrating physical prior knowledge into ML models can significantly improve prediction reliability, especially for spectral tasks.[18–20] However, few methods explicitly leverage oscillator strength—a fundamental physical quantity governing electronic transition probability—as a core descriptor.

Against this background, we propose an oscillator strength-driven ML framework (OS-ML) for λ_{max} prediction. To avoid information compression and collinearity issues with using oscillator strength as a single descriptor, we decompose it into two fundamental features: excitation energy and transition dipole moment. These are combined with molecular structural descriptors to build a hybrid feature system with clear physical significance, enabling high-precision prediction and supporting the rational design of organic optoelectronic materials.

To effectively avoid the common "black box effect" in machine learning models, this study first starts from the mechanism of predicting the absorption spectra of physically guided organic chromogenic

materials. Oscillator strength (denoted as f) is a core physical quantity used to quantitatively characterize the probability and allowance of electronic transitions from the ground state to the excited state within atoms or molecules. It is a key microscopic parameter linking molecular structure and spectral properties. The theoretical definition of oscillator strength is given in the following equation:[21]

$$f = \frac{4\pi m_e \nu}{3h} |\langle \phi_i | r | \phi_f \rangle|^2. \quad (1)$$

Here, m_e is the electron mass, ν is the molecular transition frequency, h is Planck's constant, and $\langle \phi_i | r | \phi_f \rangle$ is the transition dipole moment of the molecule from the initial state ϕ_i to the final state ϕ_f. From the formula, it can be seen that the oscillator strength physically reflects the relative transition probability of the electron transitioning from the ground state to the excited state.

According to the Franck–Condon Principle,[22] electronic transitions are not confined to the energy level corresponding to the pure electronic energy gap; instead, they can populate different vibrational energy levels of the electronic excited state, with the oscillator strength of each transition determined by its Franck–Condon factor. As shown in Fig. 1(a), when a molecule in the ground state absorbs a photon, the electron vertically transitions from the equilibrium position of the ground state (such as a_0) to a specific vibrational level on the excited state potential energy surface (such as a_1^*), rather than directly to the equilibrium position of the excited state. A single electronic transition actually corresponds to a series of vibrational transition channels, with the relative intensity of each channel determined by the square of the overlap integral of the vibrational wavefunctions (the Franck–Condon factor). This causes the absorption spectrum of isolated gas-phase molecules to exhibit a series of discrete sharp spectral lines [the yellow solid line in Fig. 1(b)], where the positions of the lines reflect the differences in vibrational energy levels, and the line intensities correspond to the relative probabilities of the various vibrational transitions. In a solution environment, due to factors such as intermolecular interactions, collisions, and solvent effects, originally sharp vibrational spectral lines become broadened. By selecting an appropriate broadening function (Gaussian functions are commonly used for electronic spectra, Lorentzian functions for vibrational spectra, and the Pseudo-Voigt function is a linear combination of the two) and combining it with the full width at half maximum (FWHM), the discrete vertical lines corresponding to oscillator strengths (with the horizontal axis representing electronic excitation energy and the vertical axis representing oscillator strength) can be broadened into continuous curves. In Fig. 1(c), the horizontal positions of the vertical lines represent electronic excitation energies, and the heights of the lines represent oscillator strengths. For example, the vertical line at 460 nm corresponds to the $S_0 \rightarrow S_5$ transition; after broadening, it becomes the green curve. The $S_0 \rightarrow S_{11}$ transition, after broadening, becomes the red curve. (Since there are many transition modes, to avoid clutter, the figure only illustrates the broadened curves for transitions with oscillator strengths greater than 0.01.) After broadening all the transitions into X-Y curves in this manner and then summing the Y values of all the curves, the resulting total curve is the black curve shown in the figure. Both experimental and theoretical studies have confirmed[23,24] that the integrated intensity of the absorption band corresponding to a single electronic transition is strictly proportional to the oscillator strength of that transition. The larger the oscillator strength value, the higher the probability of the electronic transition, and the stronger the absorption intensity of the molecule at its characteristic wavelength. This is macroscopically manifested as a higher peak value in the absorption spectrum. The magnitude of the oscillator strength determines the molecule's capacity to absorb photons at the corresponding wavelength.[25]

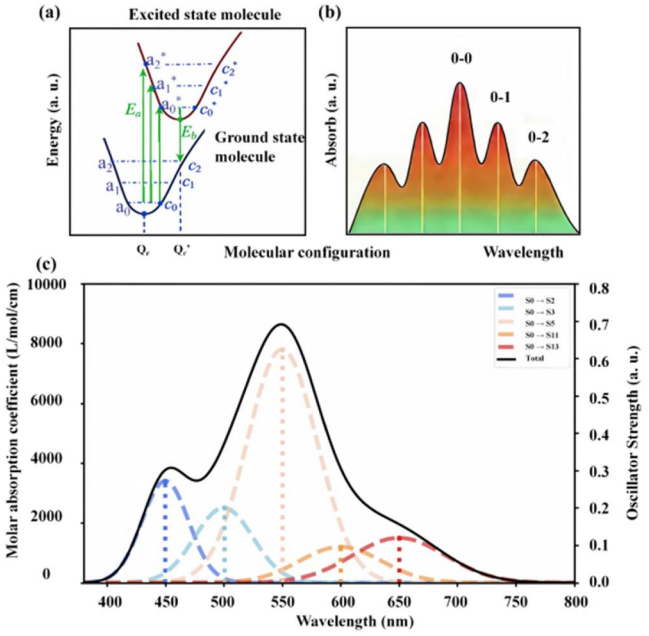

FIG. 1. Oscillator strength physical quantity and the absorption spectrum mechanism of organic materials. (a) Schematic diagram of the Franck–Condon principle and the electronic transition process. (b) Discrete vibrational spectral lines and broadened continuous absorption spectrum. (c) Broadening process of oscillator strength vertical lines into continuous absorption curves.

Therefore, based on the superior interpretability of predicting absorption spectra using the physical quantity of oscillator strength, this study establishes its quantitative structure–property relationship as a methodological framework to connect microscopic molecular design with macroscopic spectral performance. The overall process is illustrated in Fig. 2.

By exploring an oscillator strength-driven absorption wavelength prediction machine learning model (OS-ML), the aim is to develop a spectral prediction method with a clear physical mechanism and excellent predictive capability in limited-sample data scenarios.[26] To validate this scientific hypothesis, this study constructed a standardized dataset containing 74 organic chromogenic molecules, covering three typical chromogenic classes: azo, anthraquinone, and perylene derivatives. Each sample includes the molecule's three-dimensional structure and experimentally measured λ_{max}. Using Multiwfn, oscillator strengths, transition dipole moment vectors, and excitation energy calculation files of these molecules were extracted to obtain related geometric structures and solvent-related descriptors.[27] The description of the quantum chemistry calculation parameters used for the TD-DFT benchmark data can be found in the SI document. Subsequently, preliminary data organization and cleaning were performed to generate a molecular descriptor dataset.[28] The calculation

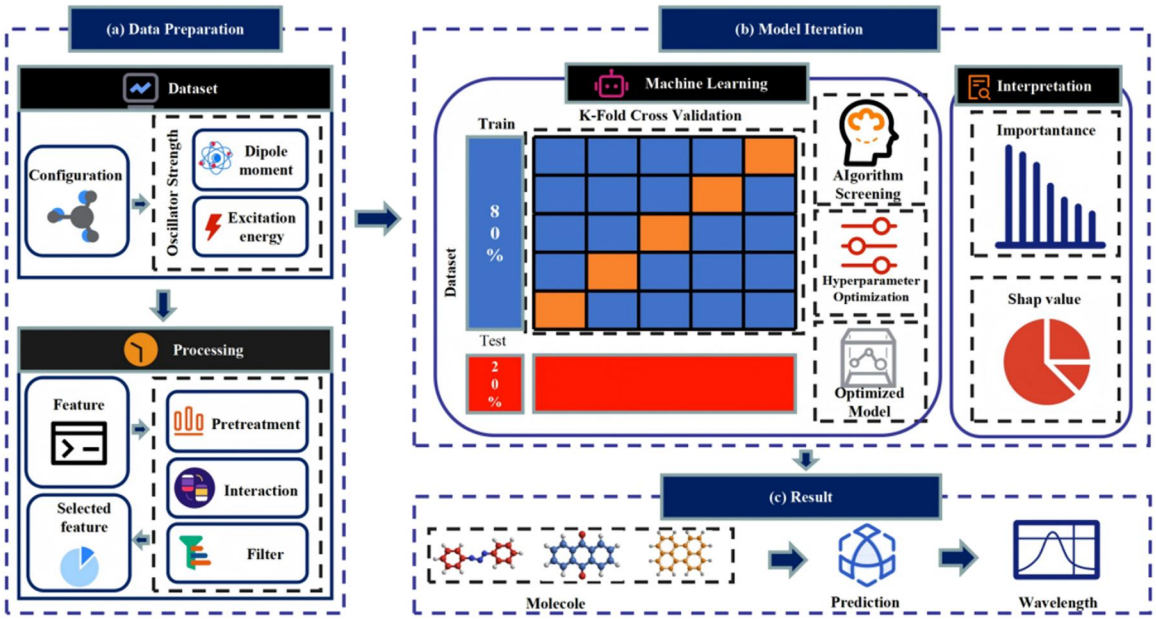

FIG. 2. Machine learning prediction framework for absorption wavelength of organic materials driven by oscillator strength. (a) Data preparation and feature engineering. (b) Model iteration and optimization. (c) Result prediction and validation.

method of molecular descriptors can be found in the supplementary material (Fig. S1). Before feature screening, oscillator strength descriptors were decomposed into two fundamental features—excitation energy and transition dipole moment—for model training.[29] Combining molecular structural features, core physical descriptors were identified as model inputs through correlation analysis and minimum redundancy maximum relevance (mRMR) selection. Finally, the prediction of the molecular λ_{max} was achieved through model selection and parameter tuning.[30,31]

To reveal the contribution of various physical descriptors to the prediction of absorption wavelengths and to verify the core role of excitation energy derived from oscillator strength and the characteristics of transition dipole moments in improving model performance, this study first constructed an initial feature set consisting of basic quantum chemical parameters and molecular structural characteristics. Through Pearson correlation analysis and mRMR feature screening methods, redundant and strongly collinear invalid features were removed, ultimately selecting core descriptors with clear physical significance as model inputs. On this basis, the SHAP method was used to perform interpretability analysis on the optimal XGBoost model. As shown in Fig. 3(a), the feature correlation heatmap verifies that there is no strong multicollinearity among the seven core descriptors selected, which not only ensures the independence and physical rationality of the model input features but also confirms the effectiveness of the feature screening method used in this study. This prevents redundant features from interfering with the model's prediction accuracy and stability from the outset. The SHAP feature importance analysis in Fig. 3(b) indicates that the excitation energy, one of the core components of oscillator strength, is the most critical factor determining the accuracy of absorption wavelength prediction, having the greatest impact on the prediction results. Another core component of oscillator strength, the transition dipole moment, together with HOMO, molecular size, and LUMO orbital delocalization index collectively form the core supporting features for the model's predictions. This directly validates the scientific rationale and necessity of introducing excitation energy and transition dipole moment as physically guided features in this study. The quantitative contribution proportions shown in Fig. 3(c) reveal that the average absolute SHAP contribution of excitation energy reaches 18.3%, ranking first among all features; the contribution of the transition dipole moment also reaches 15.3%. Together, they account for 33.6% of the total contribution, fully encompassing the core physical essence of oscillator strength and serving as the primary driving force for the model to achieve high-precision predictions.

To further verify the improvement effect of the oscillator strength-driven physically guided features on the prediction performance of the λ_{max} of organic molecules, this study compared the prediction performance of five machine learning models before and after the introduction of these features as well as the traditional TD-DFT quantum chemical calculation means on 10 independent test samples. The results are shown in Fig. 4. When the excitation energy-transition dipole moment features without the oscillator strength origin were used, the prediction results of all machine learning models found significant deviations from the experimentally measured values [Fig. 4(a)]. Among them, the support vector machine and random forest (RF) models exhibited the most severe prediction fluctuations, while the gradient boosting tree models performed relatively stably but still failed to achieve high-precision fitting of λ_{max}.

After incorporating excitation energy and transition dipole moment, which are physically rooted in oscillator strength, into the feature set, as shown in Fig. 4(b), the fit between the prediction curves of all models and the experimental benchmarks significantly

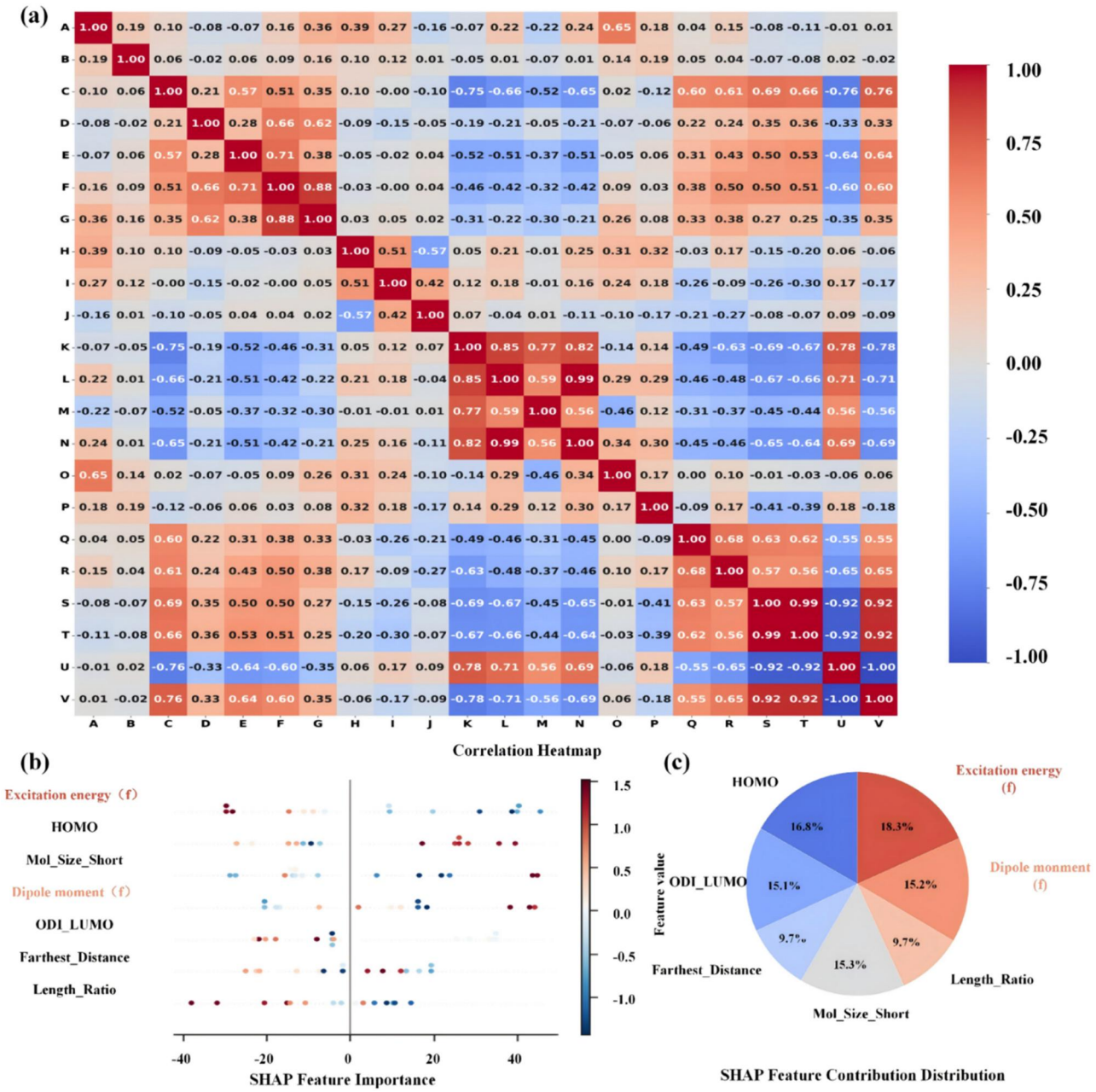

FIG. 3. SHAP interpretability analysis of core features. (a) Pearson correlation heatmap among the initial descriptors. (b) SHAP feature importance swarm plot after introducing the physical quantity of oscillator strength (decomposed into two descriptors: excitation energy and transition dipole moment). (c) Pie chart showing the proportion of average absolute SHAP contributions of each feature to the model prediction after physics-based guided selection. Mapping relationship between characters and actual molecules. For detailed information, see the supplementary material (Table S1).

improved, and the overall prediction errors were greatly reduced. Further error quantification analysis also confirmed that after introducing these core physical features, both the maximum and average prediction errors of all models decreased comprehensively, while prediction stability and generalization ability improved simultaneously. Among them, the XGBoost model achieved the best overall performance, as shown in Fig. 4(c). Compared to baseline models of the same algorithms without oscillator strength features, the machine learning models incorporating oscillator strength features reduced the MAE by more than 55%. Meanwhile, this study conducted a comparative analysis across several mainstream reference machine learning models, including Random Forest (RF), Support Vector Regression

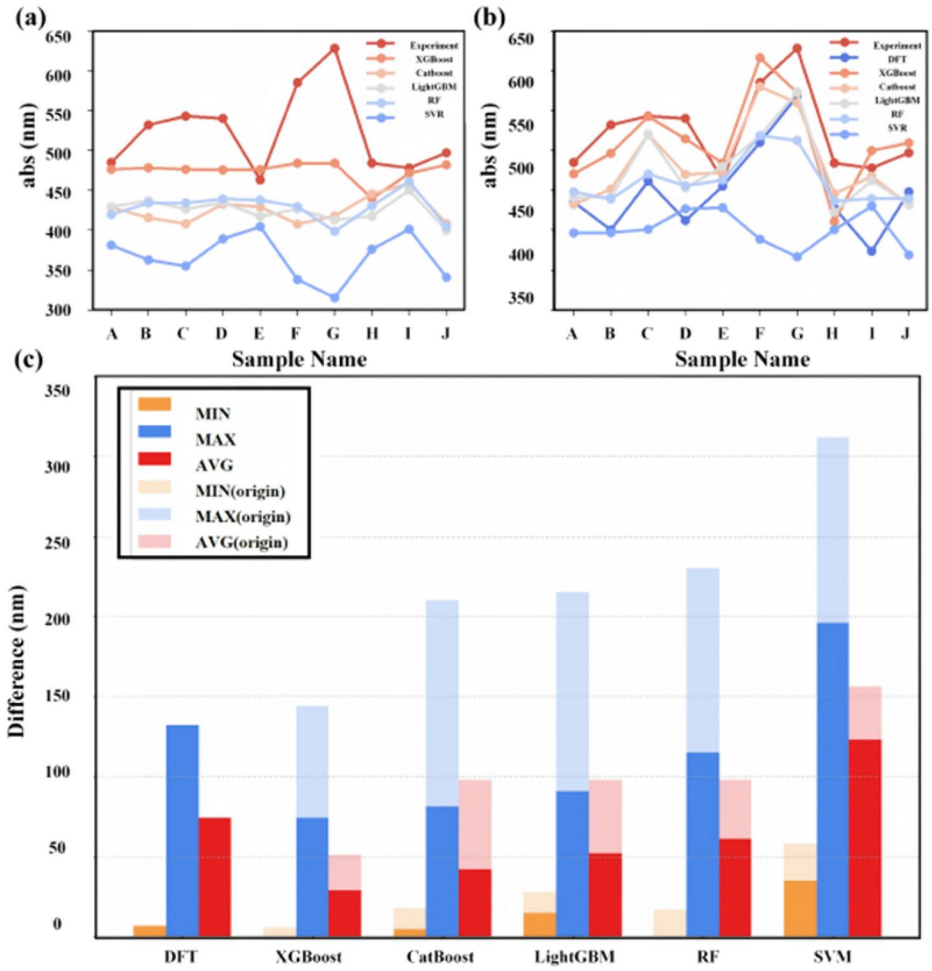

FIG. 4. Comparison of predicted λ_{max} for 10 test samples using different methods. (a) Comparison of prediction deviations between experimentally measured values and five machine learning models—XGBoost, CatBoost, LightGBM, Random Forest (RF), and Support Vector Machine (SVR)—before introducing specific features. (b) On the basis of the aforementioned machine learning models, excitation energy and transition dipole moment were introduced, followed by further comparison, including results from time-dependent density functional theory (TD-DFT) calculations. (c) Error comparison of different prediction methods before and after introducing excitation energy and transition dipole moment features. Mapping relationship between characters and actual molecules. For detailed information, see the supplementary material (Table S2).

(SVR), Light Gradient Boosting Machine (LightGBM), CatBoost as well as the XGBoost model, evaluating their comprehensive performance on the task of predicting the maximum molecular absorption wavelength λ_{max}. The results show that the XGBoost model achieved the best overall performance.

In tests on 10 independent validation samples, the coefficient of determination R^2 reached 0.89. Model hyperparameters can be found in the supplementary material document (Table S3). Compared horizontally with other reference models, the XGBoost model's MAE was reduced by more than 30% compared to the next best model, and R^2 improved by over 12%. Compared with the traditional TD-DFT quantum chemistry calculation method, this optimal model compresses the prediction time to the scale of seconds while also achieving a breakthrough in prediction accuracy by an order of magnitude. The best single-sample error can be as low as 0.6 nm, and the average prediction deviation across the entire validation set is only 40% of the TD-DFT calculation results,[32] corresponding to an approximately 2.5-fold improvement in prediction accuracy.

The aforementioned results confirm that a dual-feature system centered on oscillator strength, comprising excitation energy and transition dipole moment, can effectively compensate for the inadequacies of traditional machine learning molecular structure features in characterizing the core properties of electronic transitions. From a physical mechanism perspective, excitation energy directly corresponds to the molecular HOMO–LUMO energy gap, which fundamentally determines the energy range of electronic transitions and thereby locks in the approximate range of absorption wavelengths. This serves as the physical basis for achieving precise wavelength prediction.

The transition dipole moment is directly related to oscillator strength and can quantitatively reflect the probability of electronic transitions and absorption intensity, effectively correcting nonlinear deviations between energy gaps and wavelengths caused by different molecular structures and substituent effects. The synergistic effect of these two features addresses the issue of traditional machine learning models lacking explicit physical mechanism constraints. This is precisely the core reason why introducing these key physical features in this study significantly improved prediction accuracy and performance in limited-sample scenarios.

This study takes the oscillator strength—which directly determines the probability of electronic transitions and the core features of absorption spectra—as the physical anchor and decomposes it into

two fundamental physical characteristics: excitation energy and transition dipole moment. A hybrid feature system combining clear physical interpretability with strong predictive capability is constructed. A set of oscillator strength-driven machine learning models for predicting absorption wavelengths (OS-ML) is developed, achieving high-precision and rapid prediction of the λ_{max} of chromogenic materials. Among them, the oscillator strength-driven XGBoost model attains optimal prediction accuracy and stability. Compared with the traditional TD-DFT quantum chemical calculation methods, this model completely avoids their inherent limitations of complex computational procedures, high hardware requirements, and exponentially increasing computation time with molecular system size while achieving a breakthrough in the performance of λ_{max} prediction by orders of magnitude. This research provides a reliable new approach for efficient and high-precision prediction of optical properties and rational design of novel molecules in limited-sample scenarios, offering strong support for the targeted innovative development of organic chromogenic materials.

See the supplementary material for Figures S1–S5, Table S1, and detailed calculation methods for oscillator strength and absorption spectrum prediction.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Zijian Lin and Dechao Ye contributed equally to this paper.

Zijian Lin: Conceptualization (equal); Data curation (equal); Formal analysis (equal); Funding acquisition (equal); Investigation (equal); Methodology (equal); Project administration (equal); Resources (equal); Software (equal); Supervision (equal); Validation (equal); Visualization (equal); Writing – original draft (equal); Writing – review & editing (equal). **Dechao Ye:** Conceptualization (equal); Data curation (equal); Formal analysis (equal); Funding acquisition (equal); Investigation (equal); Methodology (equal); Project administration (equal); Resources (equal); Software (equal); Supervision (equal); Validation (equal); Visualization (equal); Writing – original draft (equal); Writing – review & editing (equal). **Jianyu Luo:** Conceptualization (equal); Data curation (equal); Formal analysis (equal); Funding acquisition (equal); Investigation (equal); Methodology (equal); Project administration (equal); Resources (equal); Software (equal); Supervision (equal); Validation (equal); Visualization (equal); Writing – original draft (equal); Writing – review & editing (equal). **Zhongshu Teng:** Conceptualization (equal); Data curation (equal); Formal analysis (equal); Funding acquisition (equal); Investigation (equal); Methodology (equal); Project administration (equal); Resources (equal); Software (equal); Supervision (equal); Validation (equal); Visualization (equal); Writing – original draft (equal); Writing – review & editing (equal). **Yan Shen:** Conceptualization (equal); Data curation (equal); Formal analysis (equal); Funding acquisition (equal); Investigation (equal); Methodology (equal); Project administration (equal); Resources (equal); Software (equal); Supervision (equal); Validation (equal); Visualization (equal); Writing – original draft (equal); Writing – review & editing (equal). **Hailing Sun:** Conceptualization (equal); Data curation (equal); Formal analysis (equal); Funding acquisition (equal); Investigation (equal); Methodology (equal); Project administration (equal); Resources (equal); Software (equal); Supervision (equal); Validation (equal); Visualization (equal); Writing – original draft (equal); Writing – review & editing (equal). **Junpeng Fan:** Conceptualization (equal); Data curation (equal); Formal analysis (equal); Funding acquisition (equal); Investigation (equal); Methodology (equal); Project administration (equal); Resources (equal); Software (equal); Supervision (equal); Validation (equal); Visualization (equal); Writing – original draft (equal); Writing – review & editing (equal). **Guofu Zhou:** Conceptualization (equal); Data curation (equal); Formal analysis (equal); Funding acquisition (equal); Investigation (equal); Methodology (equal); Project administration (equal); Resources (equal); Software (equal); Supervision (equal); Validation (equal); Visualization (equal); Writing – original draft (equal); Writing – review & editing (equal).

DATA AVAILABILITY

The data that support the findings of this study are available within the article and its supplementary material.

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