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Supporting Information

Machine learning guided full-color V_4C_3 quantum dots for building WLED

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Experimental

Materials. Nitric acid sulfuric acid was purchased from Beijing Xinbaohai Chemical Technology Co., LTD. Ethylenediamine o-phenylenediamine p-phenylenediamine sodium hydroxide was purchased from Aladdin Technology Co., LTD. Mxene nanosheets used in experimental preparation were obtained from Jilin 11 Science and Technology Co., LTD. LED chips used were purchased from Shenzhen Dongrui Technology Co., LTD With the exception of nitric acid, all chemicals were of analytical grade and did not require further purification. The ultra-pure water used in the whole experiment was prepared by BK-10B System (Dongguan Clean Environmental Protection Equipment Co., LTD.)

Characterization. Scanning electron microscopy (SEM) and energy dispersive spectroscopy (EDS) were used to scan and analyze the surface morphology of V_4C_3, and energy dispersive spectrometer was used to analyze the distribution of V and C elements in Mxene. The SEM and EDS use the NOVA Nano SEM450 field emission scanning electron microscope produced by FEI Company of the United States. The surface morphology of MQDs was studied by an atomic force microscope (AFM) after the drop mica substrate over the diluted solution was dried. The optical detection method is used to measure the change of the position of the microcantilever beam corresponding to each scanning point, so as to obtain the height change information of the surface morphology of the sample, so as to obtain the thickness of the quantum dots. The Mxene quantum dots purified after preparation were diluted 100 times with deionized water, and then dispersed evenly by ultrasound. The samples were obtained and dropped on the clean mica surface for natural drying. Fourier Transform Infrared Spectrometer (FTIR) was measured using Bruker Vertex 70 V. The dried MQDS powder was mixed with an appropriate amount of KBR powder (the mass ratio between the sample to be tested and KBR was generally 1:20), and the tablet was pressed after uniform grinding. Pure KBR powder was used as blank reference, and the scanning range was 4000-500 cm^{-1}**.**The XPS pattern was measured by Escalab 250 with monochromatic X-ray source Alkα excitation (1486.6 eV). The XPS data were calibrated with the C-C bond (284.8 eV) obtained in C1s and analyzed by X-ray diffraction spectrum using copper Kα rays at a scanning Angle of 5-90°. The photoluminescence (PL) spectra, excitation/emission curves, UV-visible absorption spectra (UV-Vis), fluorescence quantum yield (PLQY, integrating sphere) and transient fluorescence lifetime of the prepared MQDs were measured by a fluorescence spectrometer (FS5) in Edinburgh.

Synthesis of B/Y/R-MQDs. In this study, blue quantum dots (B-MQDs), yellow quantum dots (Y-MQDs) and red quantum dots (R-MQDs) were synthesized by one-step solvothermal method. In a typical process, 100 mg V4C3 Mxene is suspended in a constant temperature oil bath of concentrated sulfuric acid and nitric acid at 100°C for 12 h and the acid solution is cooled to room temperature. Slowly add sodium hydroxide aqueous solution until the pH reaches 7. The preparation process of the doped MQDs is as follows: 15 mL water and 2 mL ethylenediamine, 0.2 g o-phenylenediamine and 1.8 g p-phenylenediamine are respectively taken, and the prepared Mxene is added to a 50 mL PTFE lined stainless steel pressure cooker. The autoclave was stored at 160℃ for 12 h, 12 h and 6 h respectively, and the reaction mixture was fully separated and purified by 0.45 μm polytetrafluoron membrane filtration. The impurities were then removed by 1000 Da filtrate. The dialysis bag is dialysis for 24 hours to obtain the end product. The filtrate was then placed into a 1000 Da dialysis bag for ultra-pure water dialysis, which was updated every 10-12 hours for 2 days until no Na^+ was detected in ultra-pure water.

Preparation of WLED. The mixture of different precursor ratios B/Y/ R-MQDS and PVP was stirred for 15 minutes and then carefully dripped onto the LED chip (395nm). The bubbles are then removed with a resin vacuum extractor. Finally, the device was dried for 5h in an oven at 60℃. For white leds, a precursor ratio of 7:19:4 (volume ratio) B/Y/ R-MQDS mixture of 3 mL was mixed with 2g PVP, and the uniform mixture was then coated on the LED chip.

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Machine learning model. In the experiment, Python language was used to realize the above algorithms. The decision tree (DT) algorithm was used to judge and regression according to different features. The structure of its decision process was expanded like a tree, but its performance was poor when the input data was continuous Random forest (RF) model is to construct multiple decision trees to accomplish the data regression task together, and it is difficult to converge when the data amount is insufficient K nearest Neighbor (KNN) algorithm divides features into

K different categories according to the defined distance for learning and prediction. However, KNN model can perform well only when the data distribution is relatively uniform, and it requires rich experience to select appropriate hyperparameters, which limits the scope of application Multi-layer perceptron (MLP) algorithm uses artificial neurons to form a network to learn the feature information in the data and make predictions. However, the MLP model will have the problem of over-fitting when the data amount is insufficient.

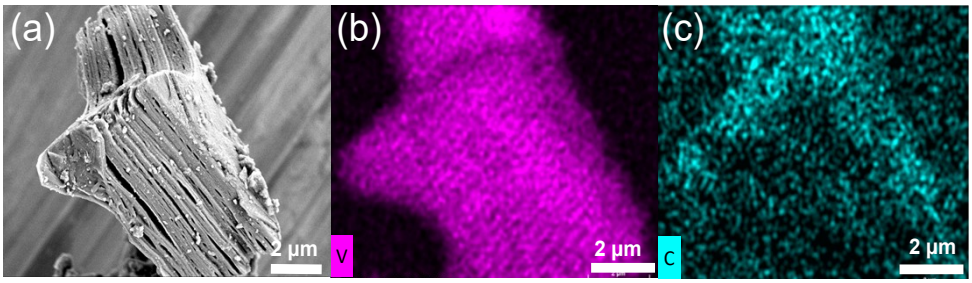

Fig. S1. (a) SEM images of V_4C_3. (b-c) V and C elemental EDX mapping analysis of V_4C_3.

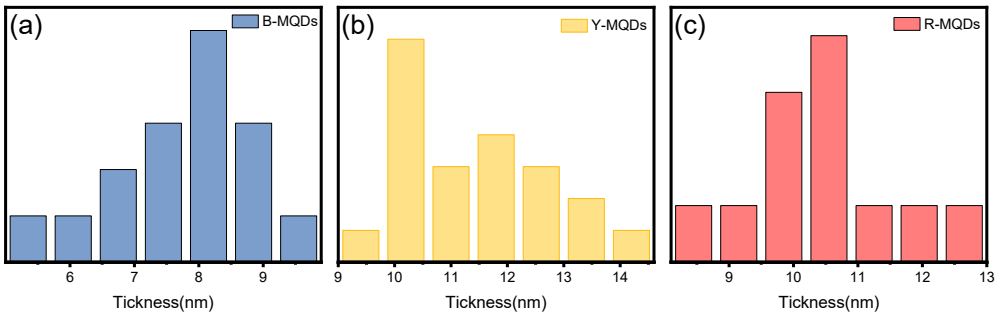

Fig. S2 Diameter size distribution of the (a)B-MQDs，(b)Y-MQDs and (c) R-MQDs.

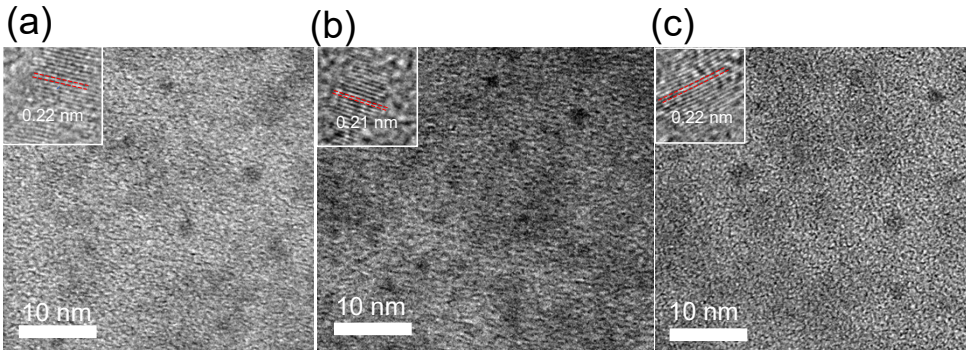

Fig. S3 TEM image of (a) B-MQDs, (b) Y-MQDs and (c) R-MQDs; (insert: HRTEM image).

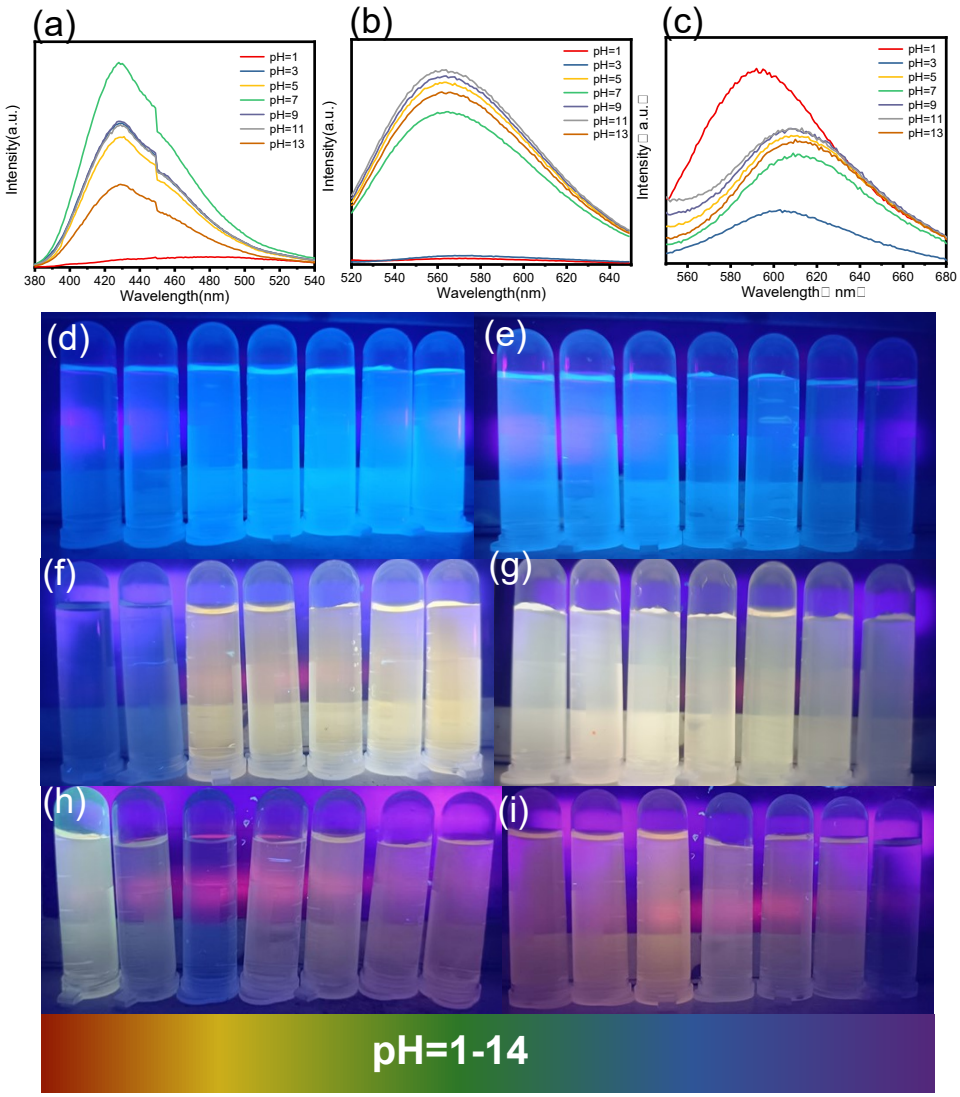

Fig. S4. pH-dependent fluorescence intensity change of the (a) B-MQDs, (b)Y-MQDs and (c) R-MQDs; pH-dependent fluorescence change photos of the (d-e) B-MQDs, (f-g) Y-MQDs and (h-i) R-MQDs.

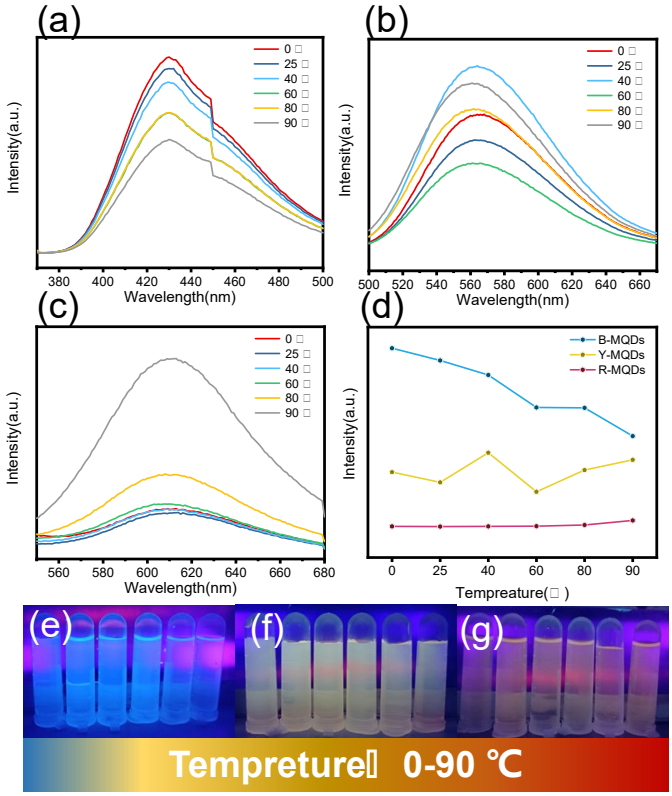

Fig. S5. Temperature-dependent fluorescence intensity change of the (a) B-MQDs，(b)Y-MQDs and (c) R-MQDs; (d) PL stability of B/Y/R-MQDs in different temperature environment**;** (e) B-MQDs, (f) Y-MQDs and (g) R-MQDs

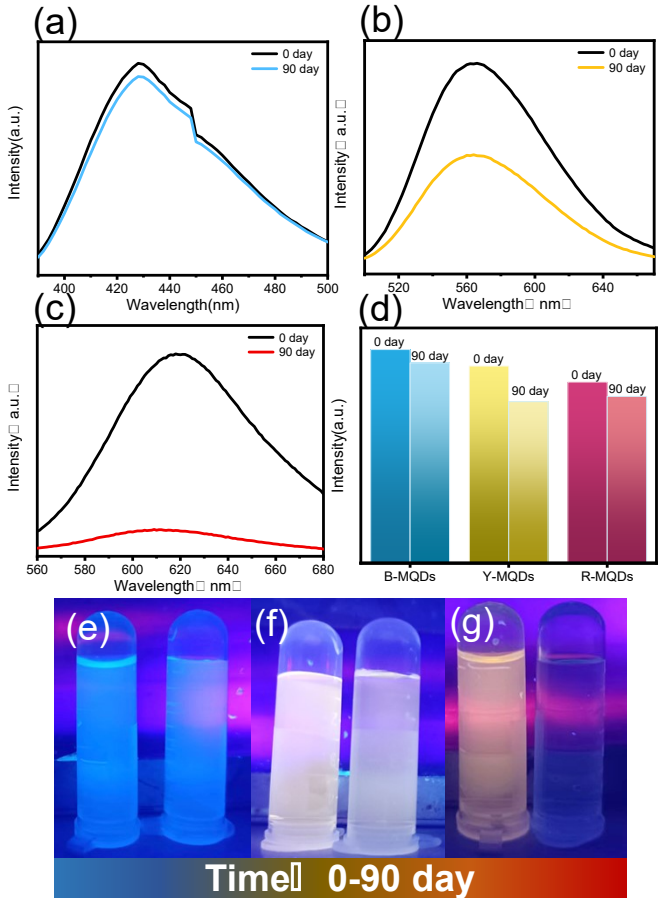

Fig. S6. Time-dependent fluorescence intensity change of the (a) B-MQDs，(b)Y-MQDs and (c) R-MQDs; (d) PL stability of B/Y/R-MQDs against time; (e) B-MQDs, (f) Y-MQDs and (g) R-MQDs

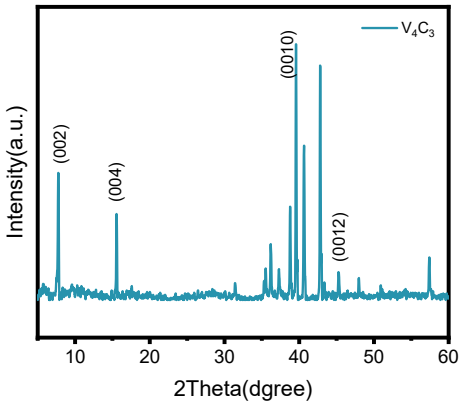

Fig. S7. XRD spectra of the V_4C_3.

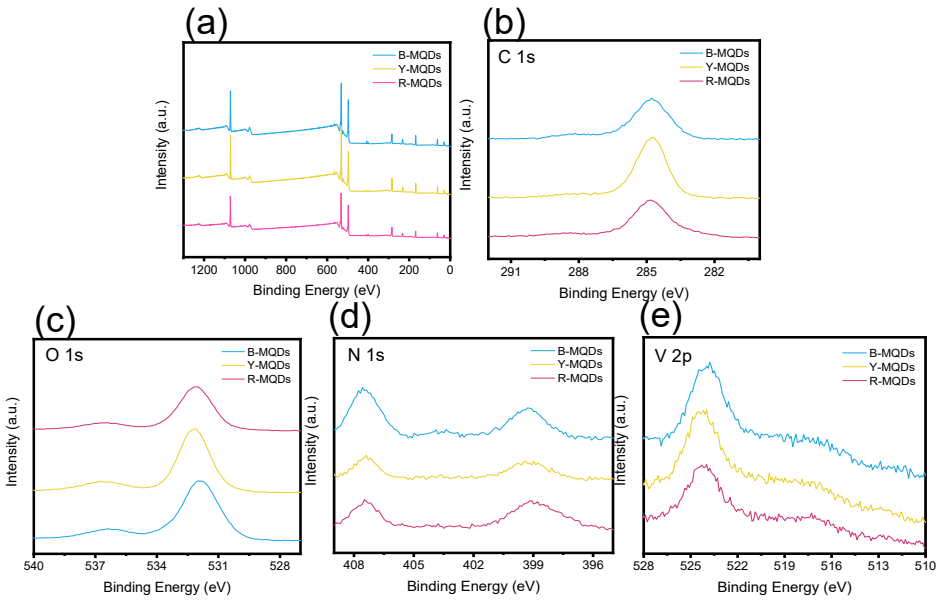

Fig. S8. XPS spectrum. (a) B/Y/R-MQDs XPS survey; (b-e) high-resolution XPS spectra of B/Y/R-MQDs.

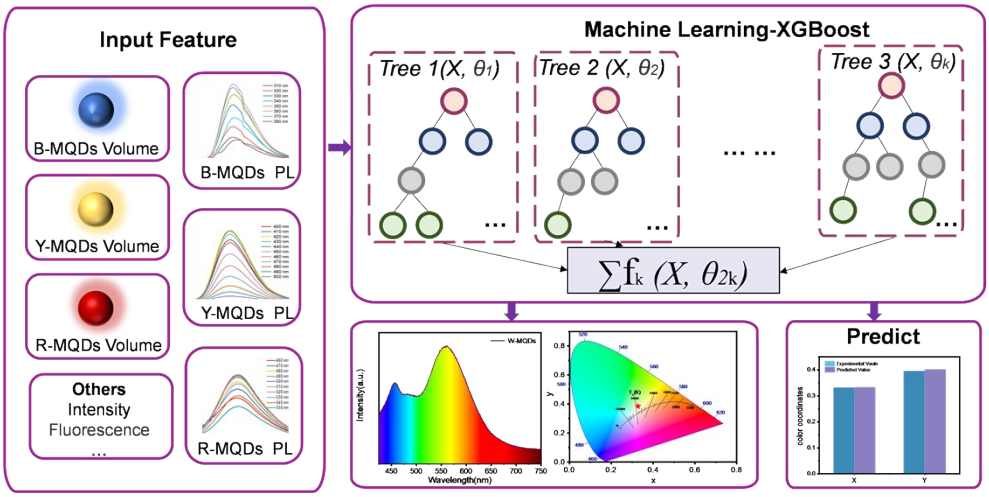

Fig. S9. Framework for the guided WLED synthesis of B/Y/R-MQDs based on ML.

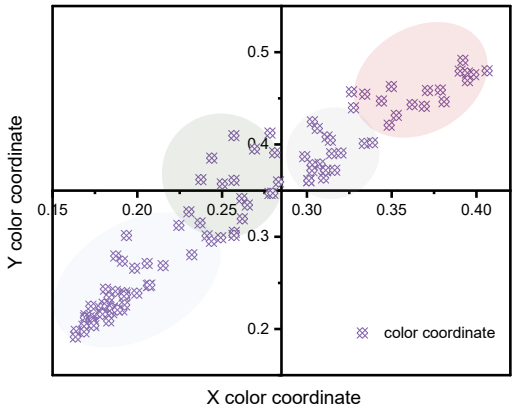

Fig. S10. The color coordinates of WLED constructed by 100 groups of B/Y/R-MQDs with different proportions.

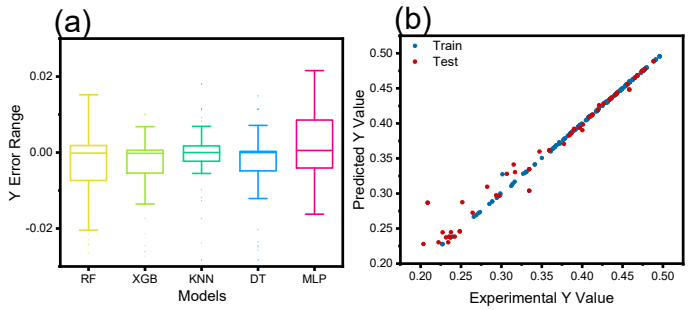

Fig. S11. (a) Error Y boxplots of RF / XGB /KNN /DT /MLP model. (b) The regression curve of training data and testing data(Y-color coordinate).

Table S1. Element content (Atomic %) of as-prepared B/Y/R-MQDs

Samples	C 1s	O 1s	N 1s	V 2p
B-MQDs	24.44	65.07	7.72	2.77
Y-MQDs	31.9	62.1	3.46	2.53
R-MQDs	28.26	63.2	5.53	2.65

Table S2. Determination coefficient R^2 and mean absolute error MAE of five candidate models (Xcolor coordinate)

Models	RF	XGB	KNN	DT	MLP
MAE	0.00693	0.00419	0.00463	0.00631	0.00708
R^2	0.9779	0.9901	0.9905	0.9773	0.9731

Table S3. Determination coefficient R^2 and mean absolute error MAE of five candidate models (Y-color coordinate)

Models	DF	XGB	KNN	DT	MLP
MAE	0.00904	0.00823	0.00685	0.00738	0.00992
R^2	0.9700	0.9721	0.9786	0.9824	0.9651