Supplementary information

Machine Learning Guided Microwave-Assisted Quantum Dot Synthesis and detection of residual H_2O_2 in human teeth

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1 Experimental

Materials. Citric acid monohydrate (99.5%) was purchased from Shanghai Hutest Laboratory Equipment Co., LTD. Ethylenediamine (99%) was purchased from Shandong West Asia Chemical Industry Co. LTD. H_2O_2 (30%) was purchased from Damao Chemical Reagent Factory. All chemicals are of analytical grade for direct use without further purification. Deionized water produced by BK-10B from Dongguanshi Qianjing environmental equipment Co, Ltd was used in all the experiments.

Synthesis of CDs. Citric acid monohydrate (0.6-1.5 g) was in dissolved deionized water (10-20 mL). The ethylenediamine (0.5-1.0 mL) was added dropwise with consistent and quick stirring. Then, the clear solution was put into a microwave oven (Galanz, P70D20TL-D4) and heated for some time at different microwave intensities. When the solution was cooled, it was filtered through a 0.22 μm polytetrafluoroethylene membrane to remove impurities to obtain the final CDs.

Machine learning models. All the code was run on the anaconda. Data was processed using the Pandas and Numpy library. The models of decision tree (DT), multilayer perceptron (MLP), random forest (RF), and XGBoost (XGB) were constructed by importing Scikit-Learn. The parameter and hyperparameter were optimized by combining the grid search algorithm and five-fold cross-validation. All of these data, code, and result can be obtained from Github. The link is https://github.com/yaoyaotang2000/ML_B-CDs.

Characterization. The morphology and microstructure of the CDs were examined by using Transmission electron microscopy (TEM) and high-resolution transmission electron microscopy (HRTEM) on a Philips Tecnai G2 F20 microscope (Philips, Netherlands) with an accelerating voltage of 200 kV. The atom force microscope (AFM) (Bruker Scan-Dimension-Icon System) was used to study the surface of the microstructure. The X-ray diffraction (XRD) was measured by Bruker D2 Phaser with an angle range from 5°to 90°. The measurement of optical character including photoluminescence, optical absorption, the photoluminescence quantum yield, and life curves used a fluorescence spectrometer (FS5) from Techcomp (China Ltd). The CD solution (30 μL) was diluted 100 times using deionized water to obtain the map of the emission spectrum. The quantum yield was measured using an FS-30 quantum yield accessory with an integrating sphere under the exaction and emission of 320 nm. The UV-Vis absorption spectra of the samples were measured using an FS-05. The FT-IR was measured on a Nicolet iS50 to characterize the functional group on the surface of CDs. The XPS was measured on the AXIS SUPRA$^+$ to analyze surface composition.

Detection of H_2O_2 using CDs. The standard solution of eight mental irons (Li^+, Mg^{2+}, Zn^{2+}, Mn^{2+}, Na^+, Cd^{2+}, K^+, Ca^{2+}) and H_2O_2 with 200 μmol/L concentration were prepared to detect the selectivity of CDs. 30 μL CDs were added into different standard solutions diluting 3 ml and were recorded with the excitation wavelength of 320 nm. Different volumes of H_2O_2 (0-1.1 M) were separately added into CDs solution and the photoluminescence intensity was recorded with the excitation wavelength of 320 nm.

2 Supplementary Figures and Tables

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2.1 Supplementary Figures

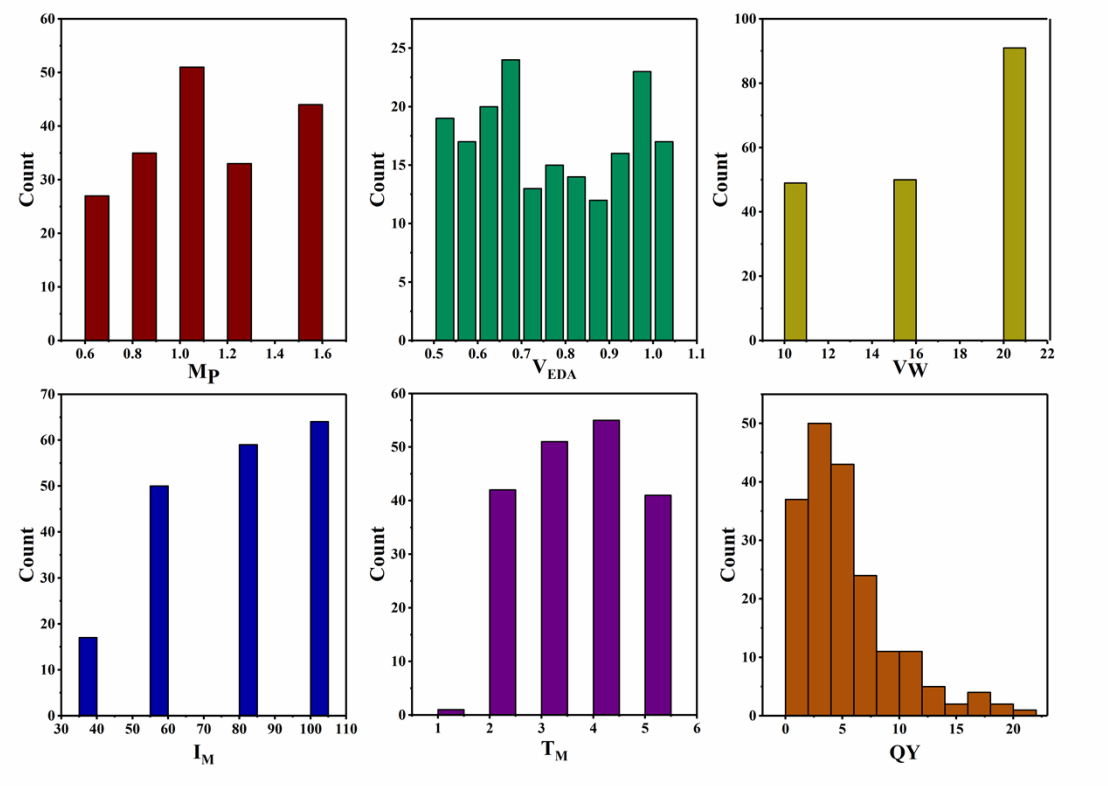

Fig S1. Histogram of microwave-assisted synthesis of CDs over each feature.

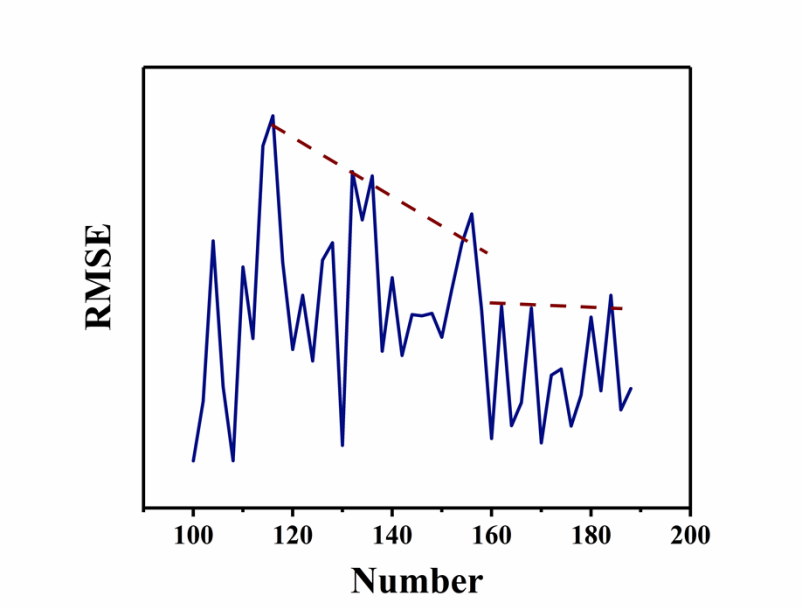

Fig S2. The performance of XGBoost vs data set ranges from 100 to 190

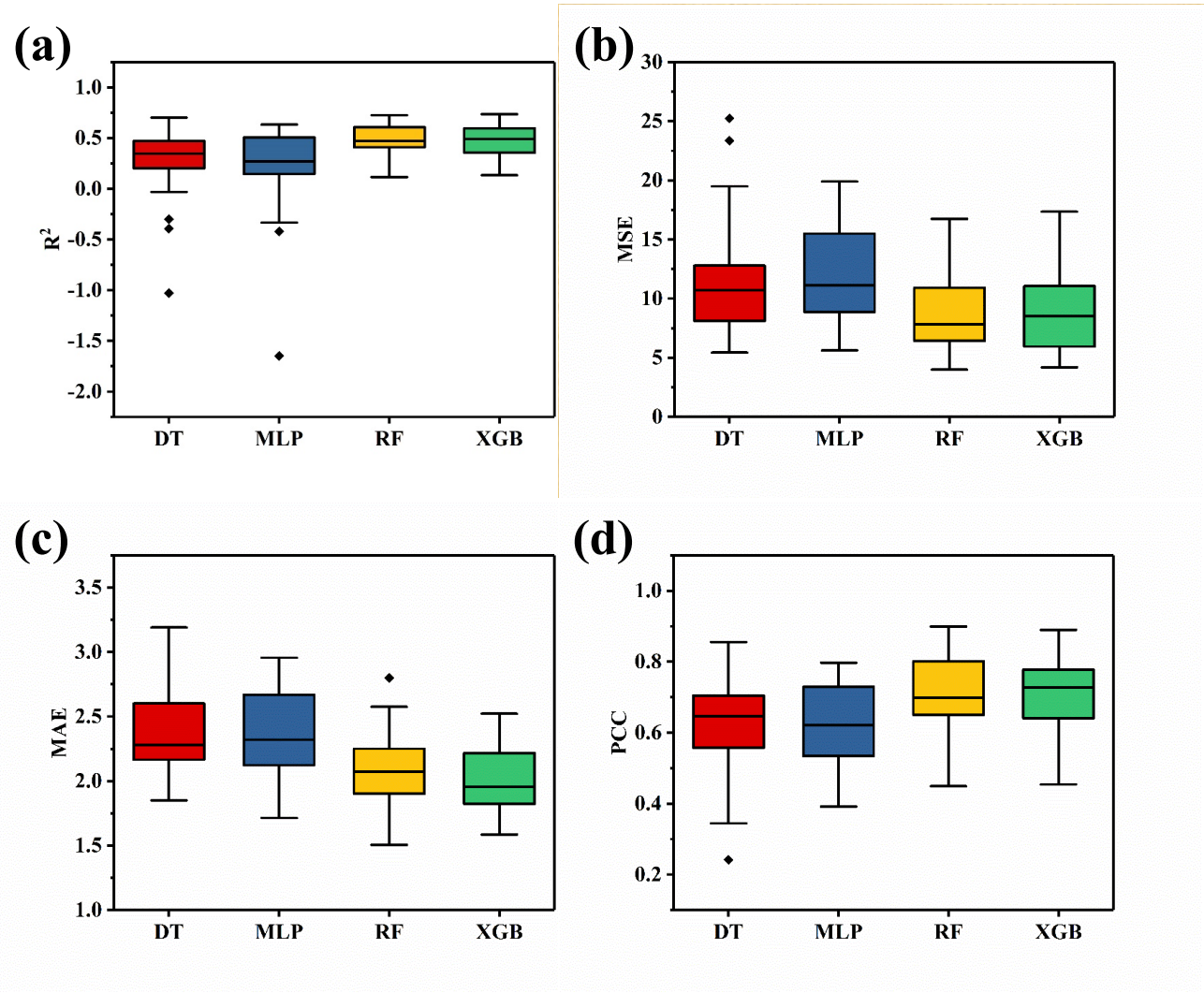

Fig S3. Boxplots among candidate models for the microwave-assisted synthesis of CDs through 6 repeatings * 5-fold cross. Red, blue, yellow, and green boxes represent the decision tree (DT), multilayer perceptron (MLP), random forest (RF), and XGBoost (XGB), respectively. (a) Boxplots compare four coefficients of mean square error (MSE). (b) Mean absolution error (MAE). (c) Coefficient of determination (R^2). (d) Pearson's correlation coefficient (PCC).

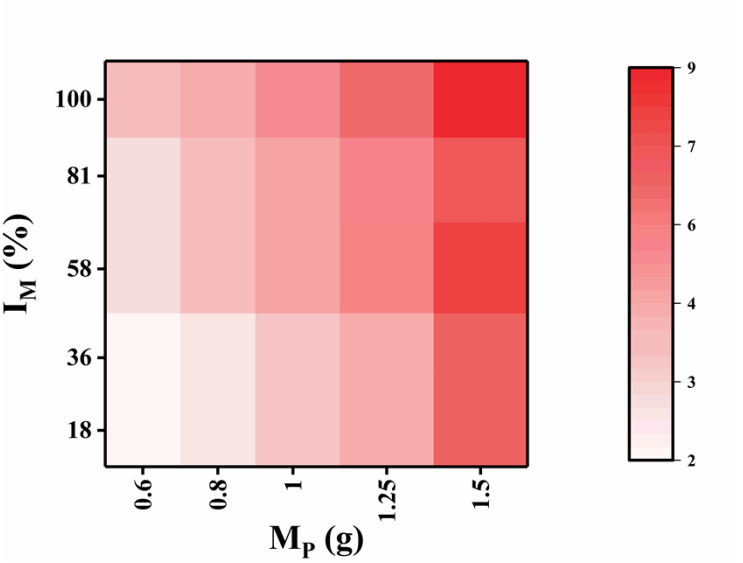

Fig S4. Predictions from the trained model, which is represented in heat map by the two most important features.

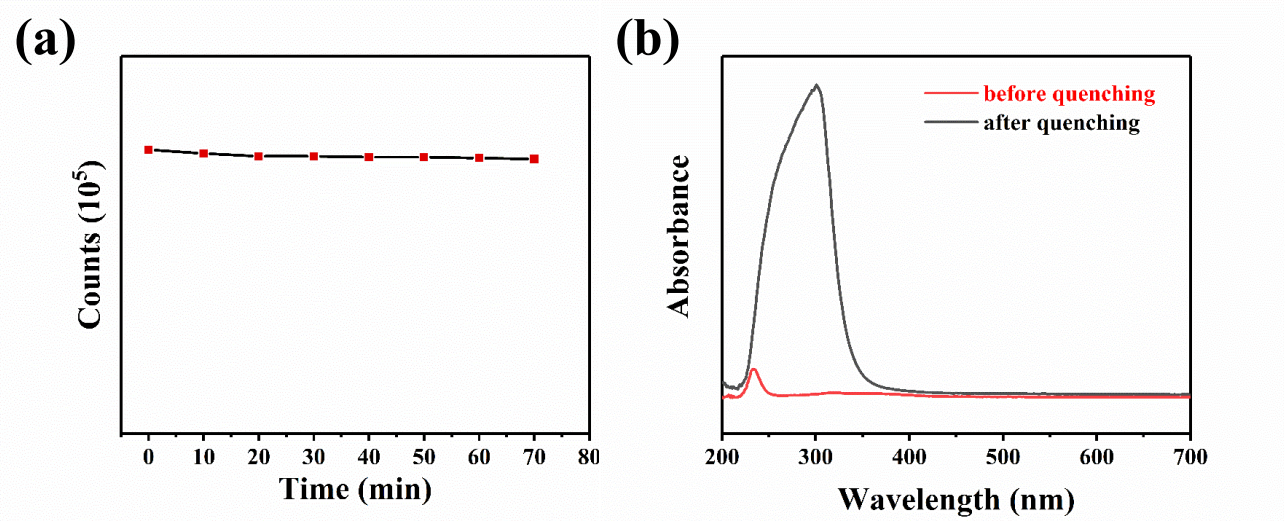

Fig S5. The stability of CDs vs times. (b) The UV-Vis absorption spectra of CDs before and after reacting with H_2O_2.

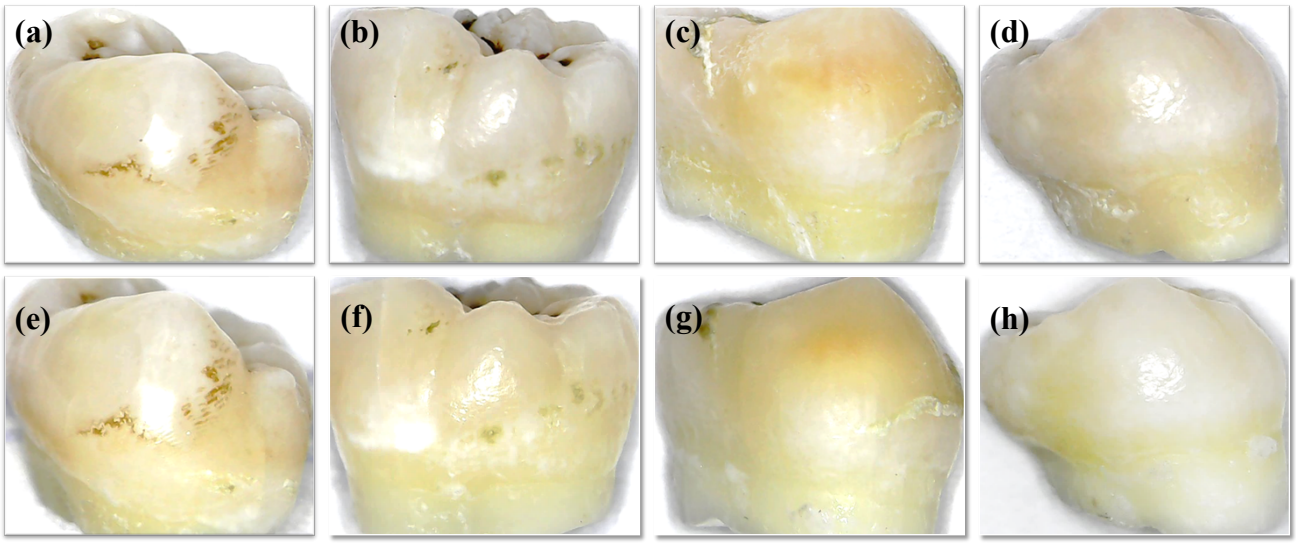

Fig S6. Photos of teeth taken before and after soaking, (a-d) the photos before soaking, (e-h) the photos after soaking. The comparison of the control group before (a) and after soaking (e) in deionized water. The comparison of the experimental group before (b) and after soaking (f) in deionized water. The comparison of the experimental group before (c) and after soaking (g) in the volume fraction of 5%. The comparison of the experimental group before (d) and after soaking (h) in the volume fraction of 10%.

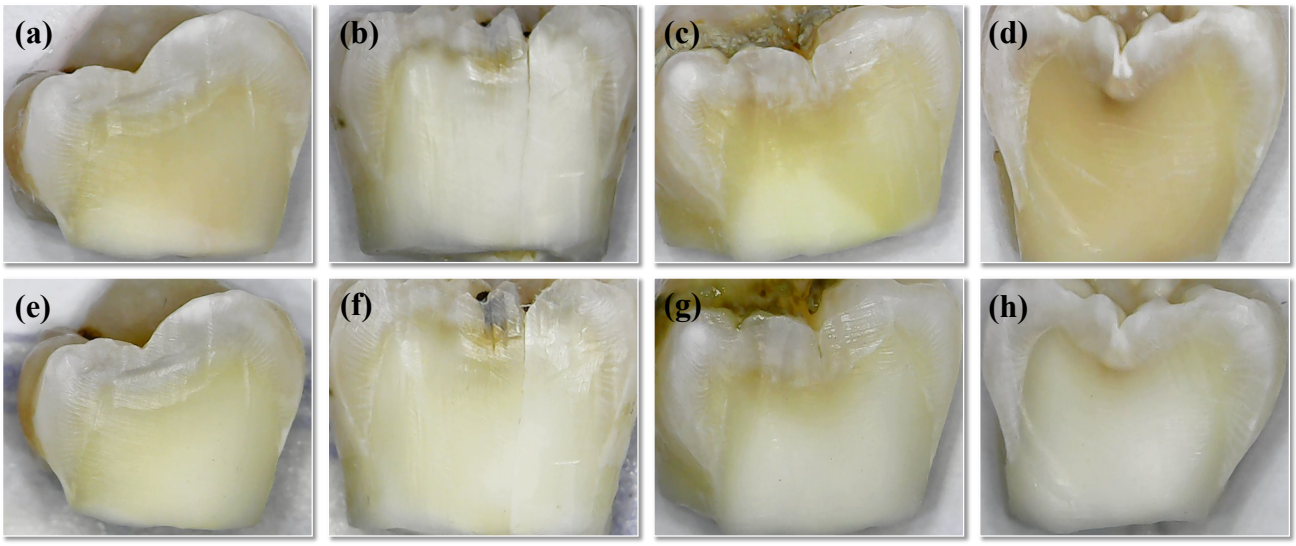

Fig S7. The photos of the polished surfaces were taken before and after soaking. (a-d) all the teeth before soaking. (e-h) All the teeth after soaking. The comparison of the control group before (a) and after soaking (e) in deionized water. The comparison of the experimental group before (b) and after soaking (f) in deionized water. The comparison of the experimental group before (c) and after soaking (g) in the volume fraction of 5%. The comparison of the experimental group before (d) and after soaking (h) in the volume fraction of 10%.

Fig S8. The fluorescence of CDs on the teeth surface after adding deionized water solution under UV light.

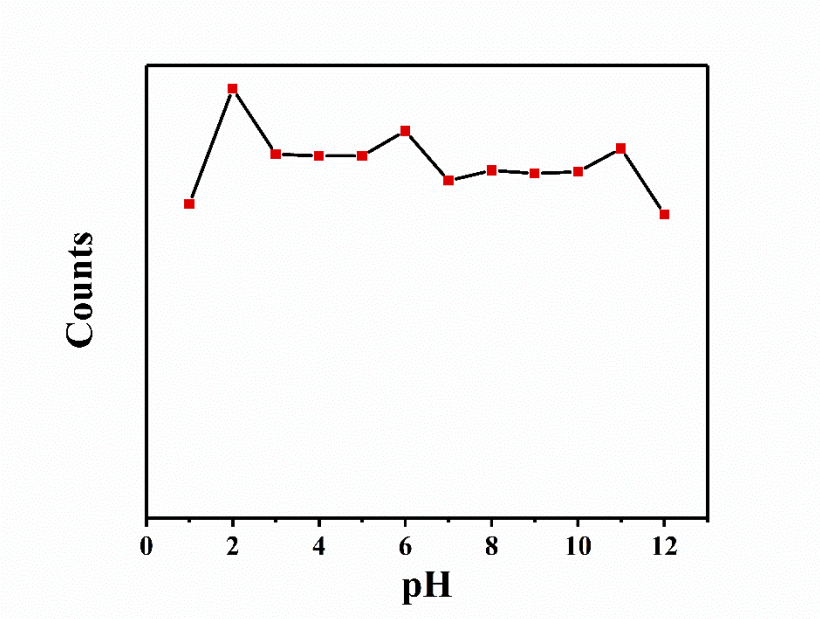

Fig S9. The stability of CDs vs pH solutions ranges from 1 to 12.

2.2 Supplementary Tables

Table S1 Five features listed above are employed to predict the QY.

Feature	Notation	Unit	Mean	Standard deviation
Mass of precursor	M_P	g	1.06	0.31
EDA volume	V_{EDA}	ml	0.74	0.16
Water volume	V_W	ml	16.10	4.16
Microwave intensity	I_M	%	77.32	20.75
Microwave time	T_M	min	3.49	1.08
Quantum yield	QY	%	5.25	4.17

Table S2 Change range and increment value of five input parameters

Parameter	Min	Max	Increment
Mass of precursor (g)	0.6, 0.8, 1.0, 1.25, 1.5		
EDA volume (ml)	0.5	1.0	0.05
Water volume (ml)	10	20	5
Microwave intensity (%)	18, 36, 58, 81, 100		
Microwave time (min)	2	5	1

Table S3 The elements ratio of CDs in the XPS survey spectrum.

elements	C	N	O
Percentage (%)	66.27	10.41	23.32