**Supplementary material**

**Preparation and evaluation of poplar waste derived adsorbent for dye**

**removal：adsorption mechanism and DFT calculation**

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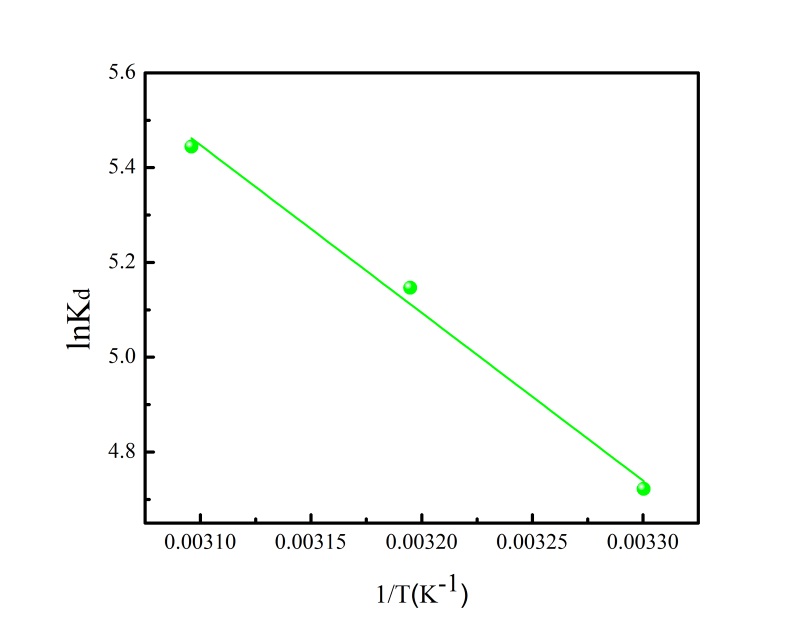
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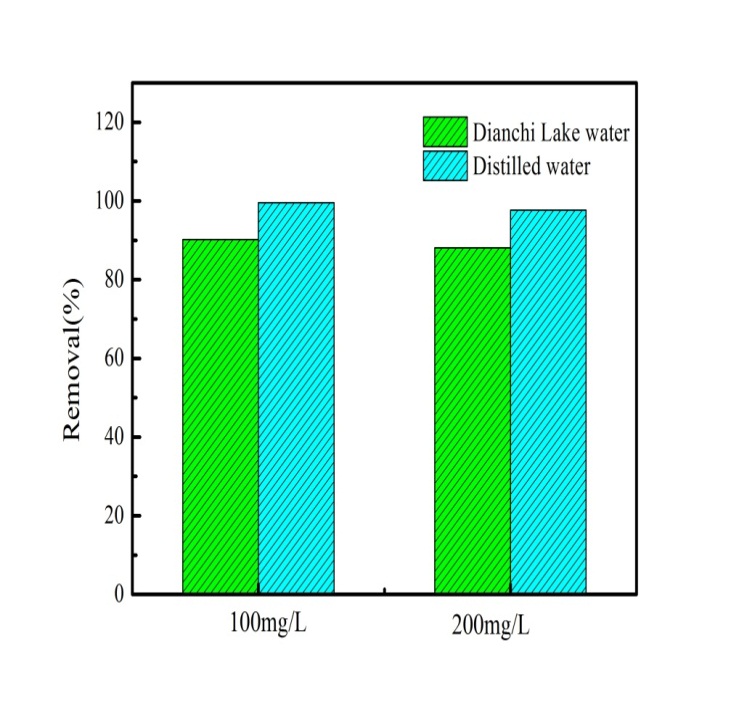
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**Fig.S1** The slope and intercept of ln (Kd) vs. 1/T plot.

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**Fig.S2** Reusability of PWA for MB adsorption.



**Fig.S3** Comparison of MB removal on PWA in actual water and distilled water

**Table S1** Adsorption isotherm models adopted in this work and their parameters.

|  |  |  |
| --- | --- | --- |
| Isotherm | Equation | Parameters |
| Langmuir |  | Ce is the equilibrium concentration(mg/L)  Q0 (mg/g) is adsorption constant related to adsorption capacity  KL (L/g) is adsorption constant related to energy of adsorption |
| Freundlich |  | KF is adsorption constant related to adsorption capacity (mg/g).(L/mg)1/n  n is adsorption constant measuring the adsorption intensity |
| Dubinin-Radushkevich |  | α is the adsorption capacity(mg g-1)  β is the constant related to the adsorption energy (mol2kJ-2) |
| Temkin |  | A and B are constants |

**Table S2** Adsorption kinetic models adopted in this work and their parameters.

|  |  |  |
| --- | --- | --- |
| Kinetic models | Equation | Parameters |
| Pseudo-first order |  | qe is the uptake of methylene blue at equilibrium (mg/g).  K1 (1/min) is the adsorption rate constant, |
| Pseudo-second order |  | K2 (g/mg min) is the rate constant of second-order equation |
| Intraparticle diffusion |  | K3 (mg/g min1/2) is the intraparticle diffusion rate constant  C is a constant |
| Elovich |  | a (mg/g min) is the initial adsorption rat  b (g/mg) is related to the extent of surface coverage and activation energy. |

**Table S3** Fixed bed models and corresponding parameters.

|  |  |  |
| --- | --- | --- |
| Model | Equations | Parameters |
| Thomas |  | *KTh* (mL min-1 mg-1) is the Thomas constant, *qth* (mg g-1)is the maximum adsorption capacity, *M* (mg) is the weight of ZnFe-BC, *V* (mL min-1) is the inlet flow. |
| Yoon-Nelson |  | KYN (min-1) is the Yoon-Nelson constant and t0.5 (min) is the time required for 50% breakthrough. |