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SWCNT functionalised with poly(vinyltriazole): a method to determine the optimal stoichiometry through adsorption kinetics and isotherms

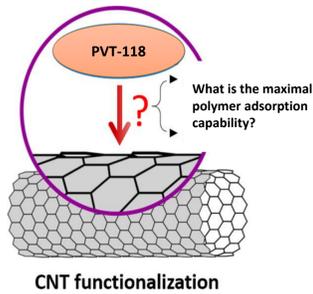
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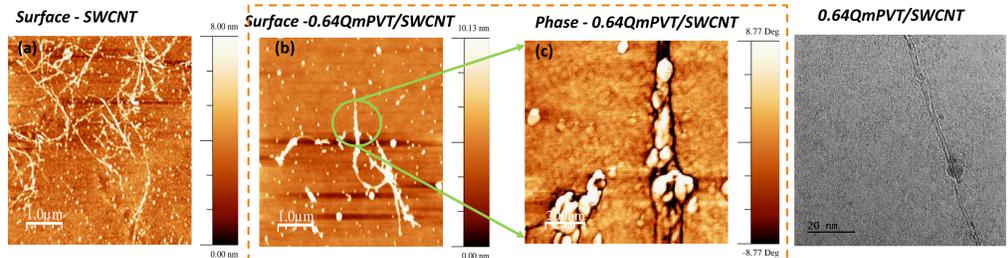
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1. Why the study of Polymer:SWCNT stoichiometry is important for optoelectronic applications?

- Excess of polymer compared to the available CNT binding sites leads:
 - Polymer aggregation by intermolecular coiling
 - Low electrical performance due to high contact resistance
- Excess of SWCNT leads to free binding sites
 - Lack of sensitivity
 - Lack of selectivity

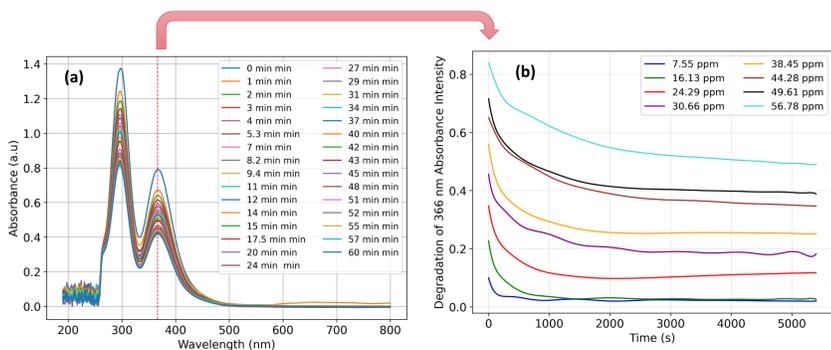


2. 1 Surface Morphology



- TEM diameter of SWCNT is 0.60 nm
- TEM diameter of 0.64QmPVT/SWCNT is 2.79 nm

2.2. Evolution of Absorbance as a function of time



- Absorption spectra of PVT-118 (a) show two peaks at 295 nm (assigned to the poly(vinyl) chain) and 366 nm (assigned to the triazole groups)
- 366 nm peak is a good marker because PVT-118 interacts with SWCNT through the triazole groups by π -stacking

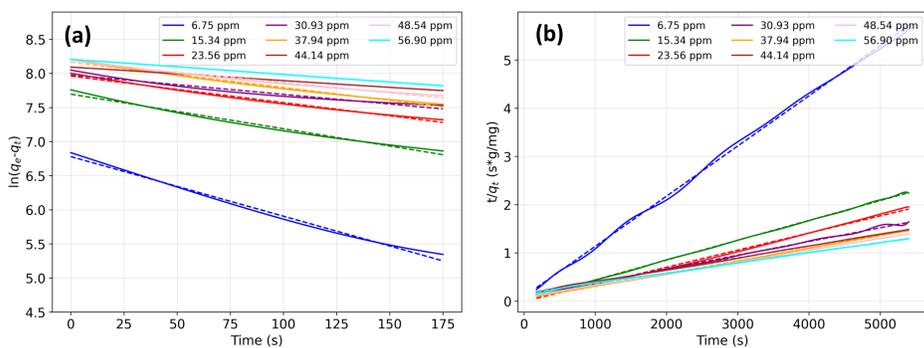
2.3 Kinetics models for understanding the dynamics

Pseudo-first-order kinetics model

$$\ln(q_e - q_t) = \ln q_e - k_1 t$$

Pseudo-second-order kinetics model

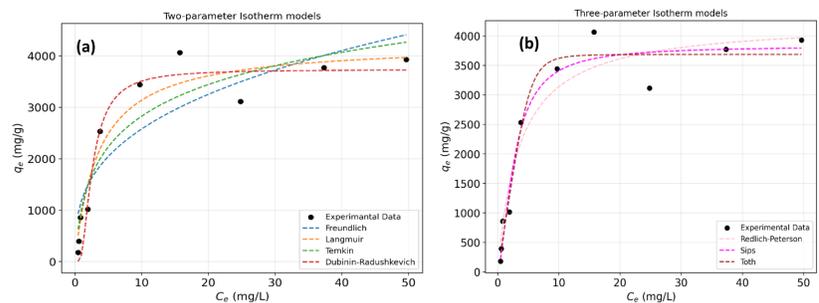
$$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \left(\frac{1}{q_e}\right) t$$



- q_e - mass of polymer at equilibrium per unit mass of SWCNT ($mg \cdot g^{-1}$)
- q_t - mass of polymer at time t per unit mass of SWCNT ($mg \cdot g^{-1}$)
- k_1 - first-order adsorption rate constant (s^{-1})
- k_2 - second-order adsorption rate constant ($g \cdot mg^{-1} \cdot s^{-1}$)
- t - time (s)
- C_0 - Initial concentration (mg/L)
- C_t - Concentration at time t (mg/L)
- m - mass of the adsorbent (g)
- V - Volume of the dynamic system (L)

- Before 175s, 1st-order kinetics \rightarrow process governed by availability of free binding sites
- After 175s, 2nd-order kinetics \rightarrow process governed by rarity of binding sites

2.4 Isotherm Models for understanding the surface coverage



Name of the Isotherm model	Name of the parameter	Value	R ²	MAPE
Freundlich	$K_f (mg/g)$	1191	0.82	76%
Langmuir	$q_m (mg/g)$	4324	0.94	35%
Temkin	$K_{Te} (Lg^{-1})$	2.1	0.89	48%
Dubinin-Radushkevich	$q_m (mg/g)$	3733	0.93	34%
Redlich-Peterson	$K_R (L/g)$	1195	0.94	35%
Sips	$q_m (mg/g)$	3828	0.96	16%
Toth	$q_m (mg/g)$	3684	0.96	18%

MAPE – Mean absolute percentage error

- The calculated C_e values for the plot isotherms were covered by first order and second order kinetic part

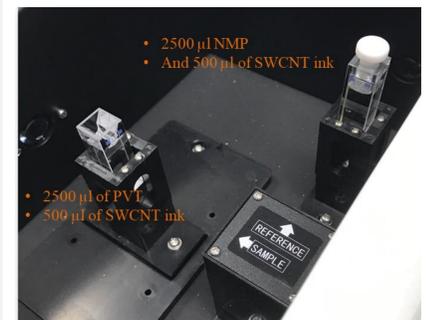
$$q_e = \frac{(C_0 - C_e)}{m} V$$

q_e - Equilibrium adsorption capacity (mg/g)
 C_e - Equilibrium concentration (mg/L)

- Maximum surface coverage obtained from the Toth isotherm model (Q_m) is 3684.5 mg/g

3. UV-Vis spectrophotometer based Methodology for adsorption Kinetics and Isotherm analysis on solution phase SWCNT ink

- 1st step - Automatic Zero calibration with NMP (solvent) in both cuvette
- 2nd step - Reference cuvette with the NMP (2500 μ l) + SWCNT ink (500 μ l)
- 3rd step - Sample cuvette filled with the PVT polymer (2500 μ l) + SWCNT ink (500 μ l) and run the kinetics studies



4. Conclusion

- PVT-118 and SWCNT functionalization demonstrated by mix order kinetics
- Multilayer adsorption process follow the Toth Isotherm model
- The calculated Maximum surface coverage (Q_m) by the Toth Isotherm model is 3684.5 mg/g

5. Acknowledgment

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6. Bibliography

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