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

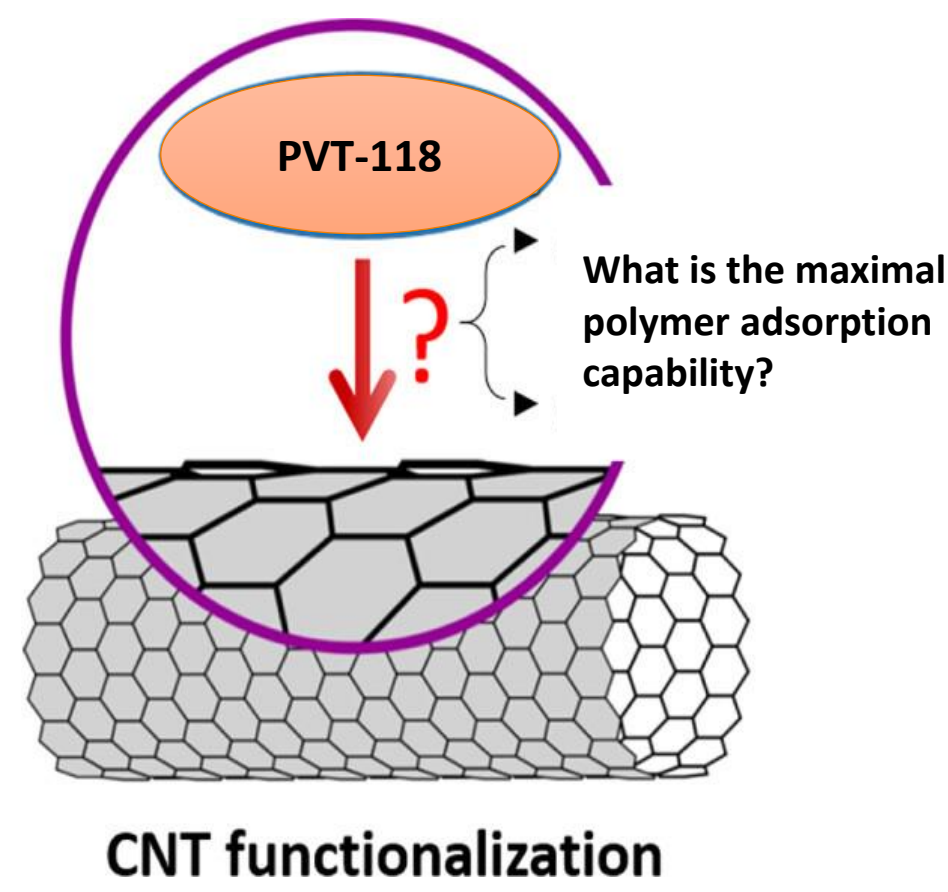
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<sup>1</sup> IMSE (Laboratoire Instrumentation, Modélisation, Simulation Et Experimentation) - Université Gustave Eiffel

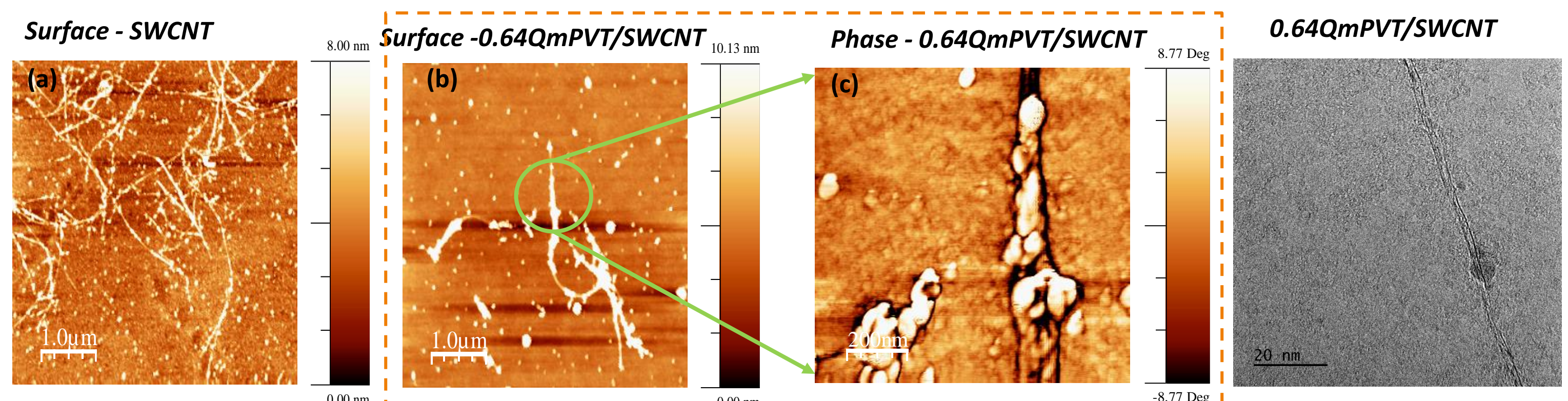
<sup>2</sup> ITODYS (Interfaces – Traitement – Organisation et Dynamique des Systèmes) – Université Paris Cité

## 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

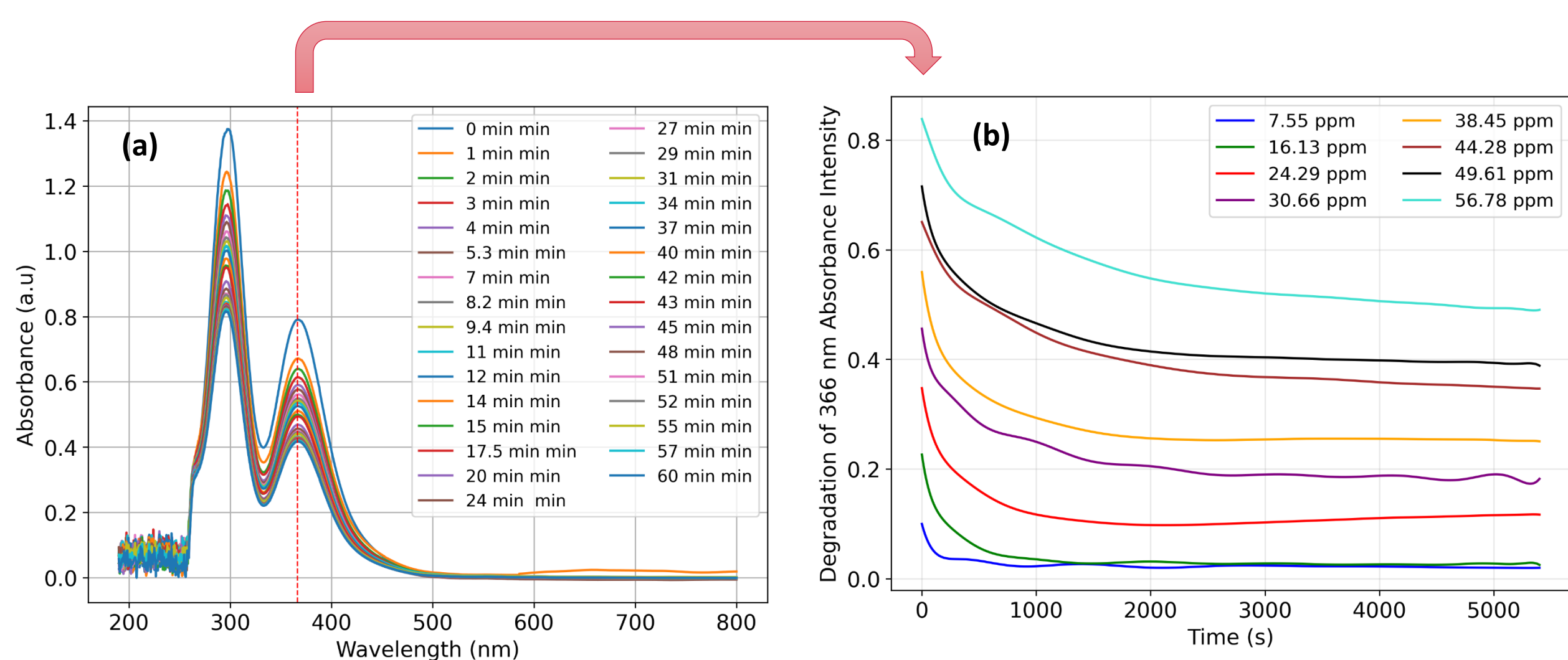


## 2. 1 Surface Morphology



- 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  $\pi$ -stacking

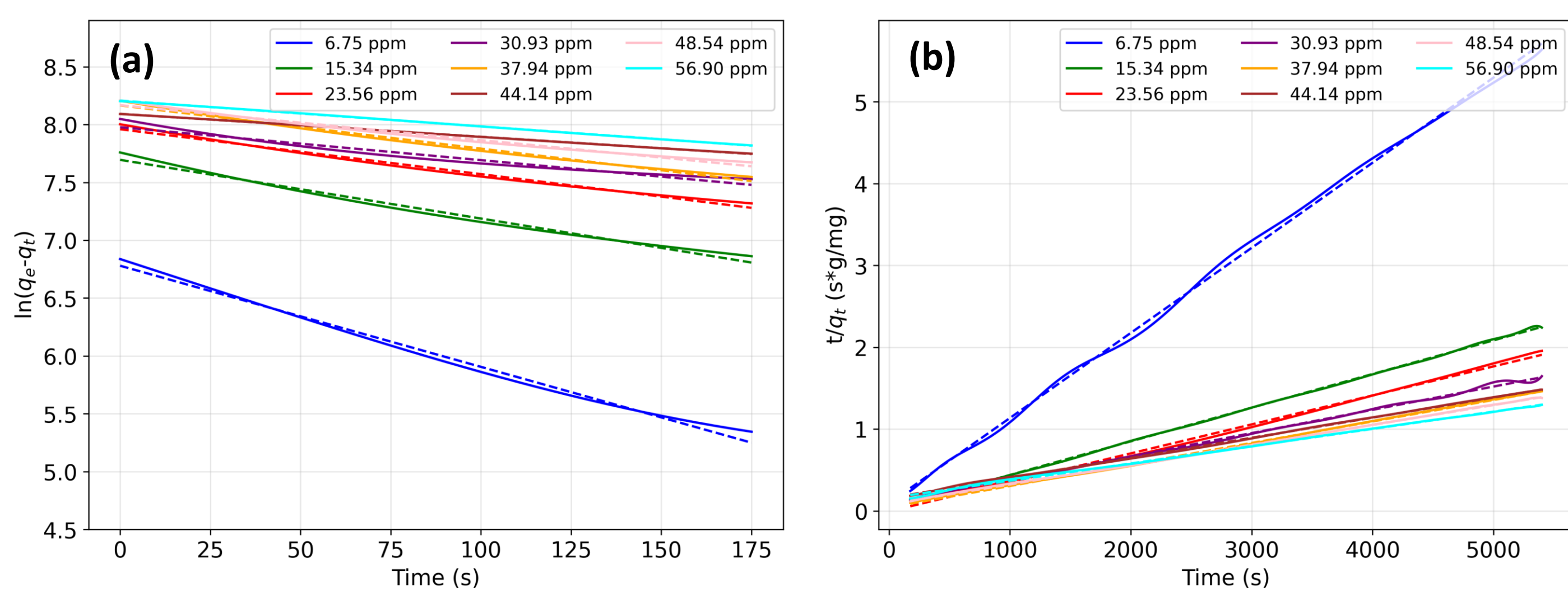
## 2.3 Kinetics models for understanding the dynamics

### Pseudo-first-order kinetics model

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

### Pseudo-second-order kinetics model

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

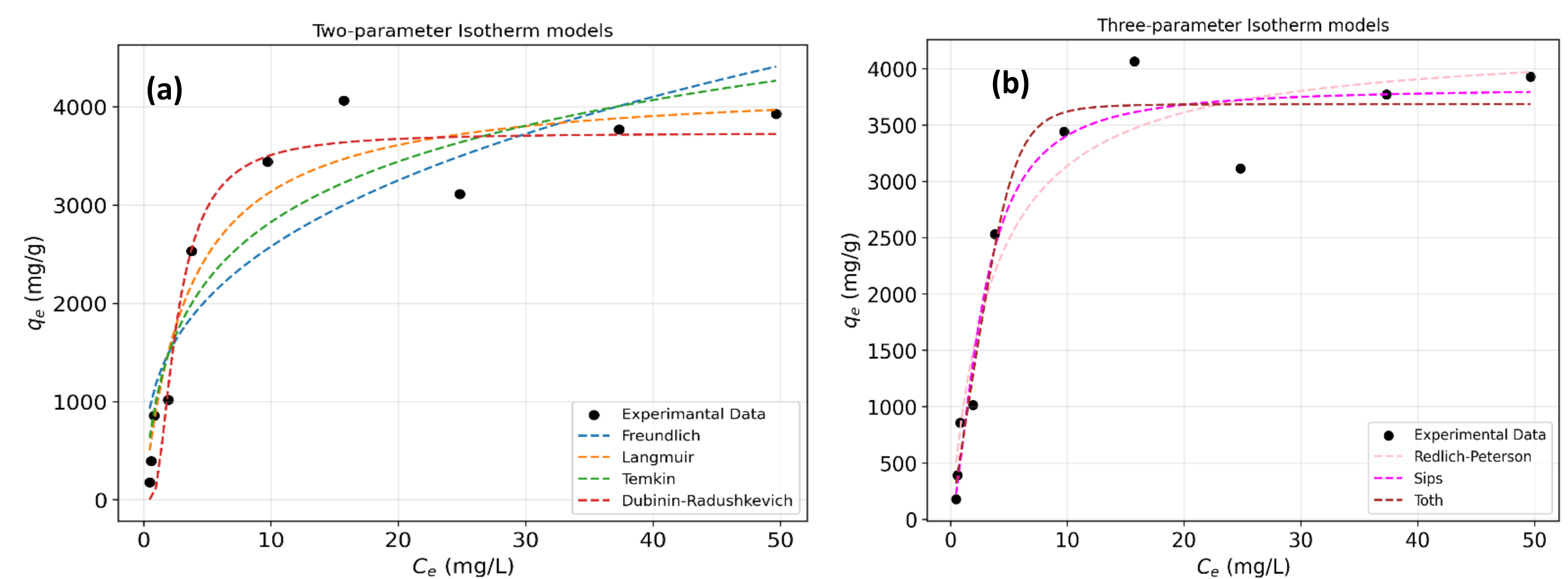


- $q_e$  - mass of polymer at equilibrium per unit mass of SWCNT ( $mg \cdot g^{-1}$ )
- $q_t$  - mass of polymer at time  $t$  per unit mass of SWCNT ( $mg \cdot g^{-1}$ )
- $k_1$  - first-order adsorption rate constant ( $s^{-1}$ )
- $k_2$  - second-order adsorption rate constant ( $g \cdot mg^{-1} \cdot s^{-1}$ )
- $t$  - 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)

$$q_t = \frac{(C_0 - C_t)}{m} V$$

- Before 175s, 1<sup>st</sup>-order kinetics  $\rightarrow$  process governed by availability of free binding sites
- After 175s, 2<sup>nd</sup>-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 <sup>2</sup>	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

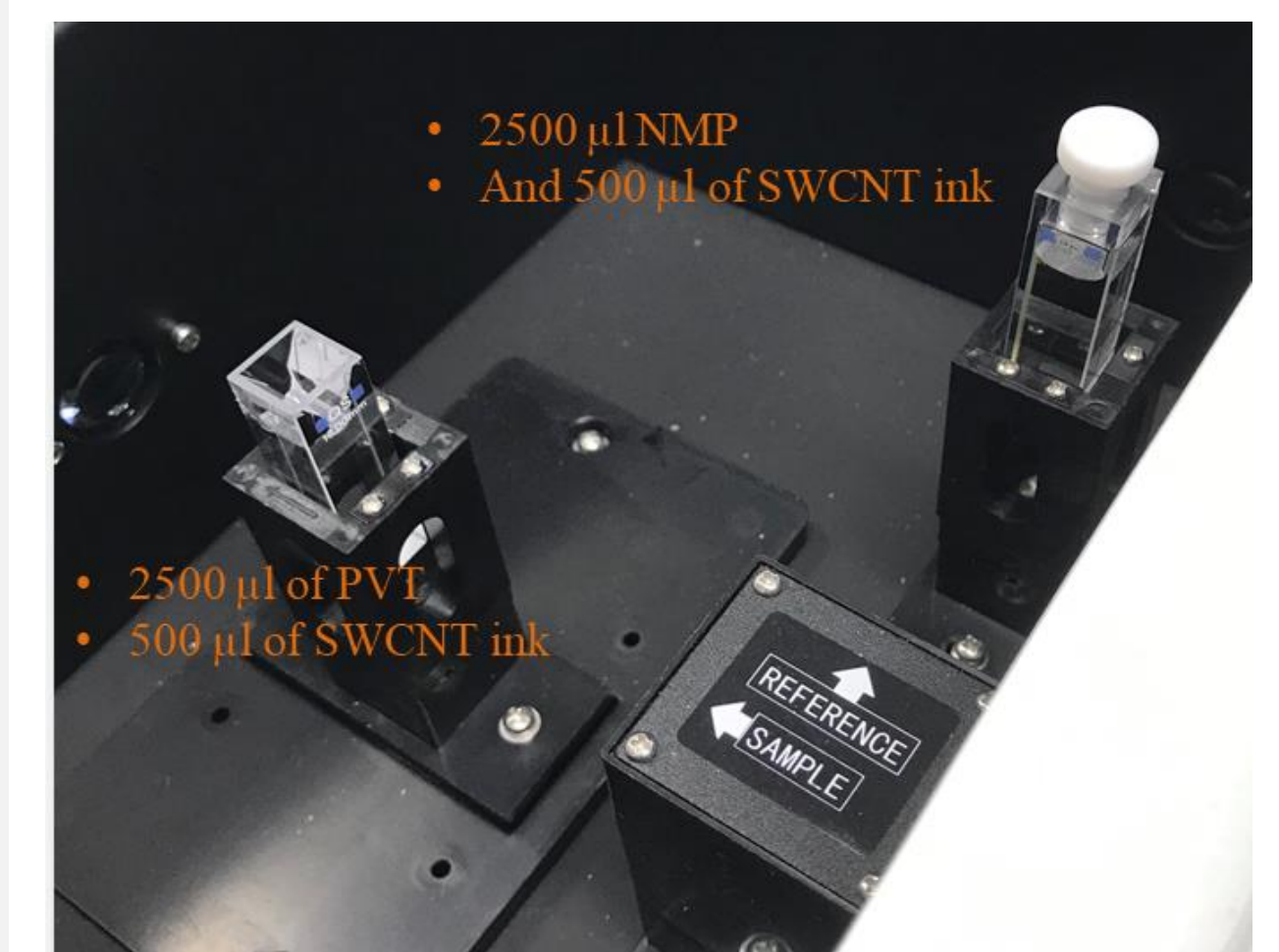
$$q_e = \frac{(C_0 - C_e)}{m} V$$

$q_e$  - Equilibrium absorption 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

- 1<sup>st</sup> step - Automatic Zero calibration with NMP (solvent) in both cuvette
- 2<sup>nd</sup> step - Reference cuvette with the NMP (2500  $\mu$ l) + SWCNT ink (500  $\mu$ l)
- 3<sup>rd</sup> step - Sample cuvette filled with the PVT polymer (2500  $\mu$ l) + SWCNT ink (500  $\mu$ 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

Al-Ghouti, M. A., & Da'ana, D. A. (2020). Guidelines for the use and interpretation of adsorption isotherm models: A review. Journal of Hazardous Materials, 393, 122383. <https://doi.org/10.1016/j.jhazmat.2020.122383>