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Molecular-Level Dispersion of Pristine Graphene in Water via Polymer Physisorption

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Abstract: Doping high amounts of graphene into polymer matrixes is desirable for producing multifunctional nanocomposites with improved mechanical strength and electrical conductivity.[1] Using liquid-phase exfoliation, polymers can assist graphene dispersion, which is generally attributed to steric forces that form between adsorbed polymers in graphene.[2] In this study, we demonstrated that well-dispersed graphene concentrations can be manipulated in water using varying concentrations of polyvinyl alcohol. Based on Flory's classic theory, we first proposed a model to describe the polymer adsorption process in graphene/polymer/solvent ternary systems in a "dilute" regime and simulated the adsorption-free energy changes during this transformation. More specifically, we demonstrated that the adsorption is influenced by the different affinities among graphene, polymer, and solvent and by the polymer's molar weight. These results increase our fundamental understanding of the polymer physisorption of 2D materials and introduce a new method of producing 2D material-based polymer nanocomposites.

Experiental

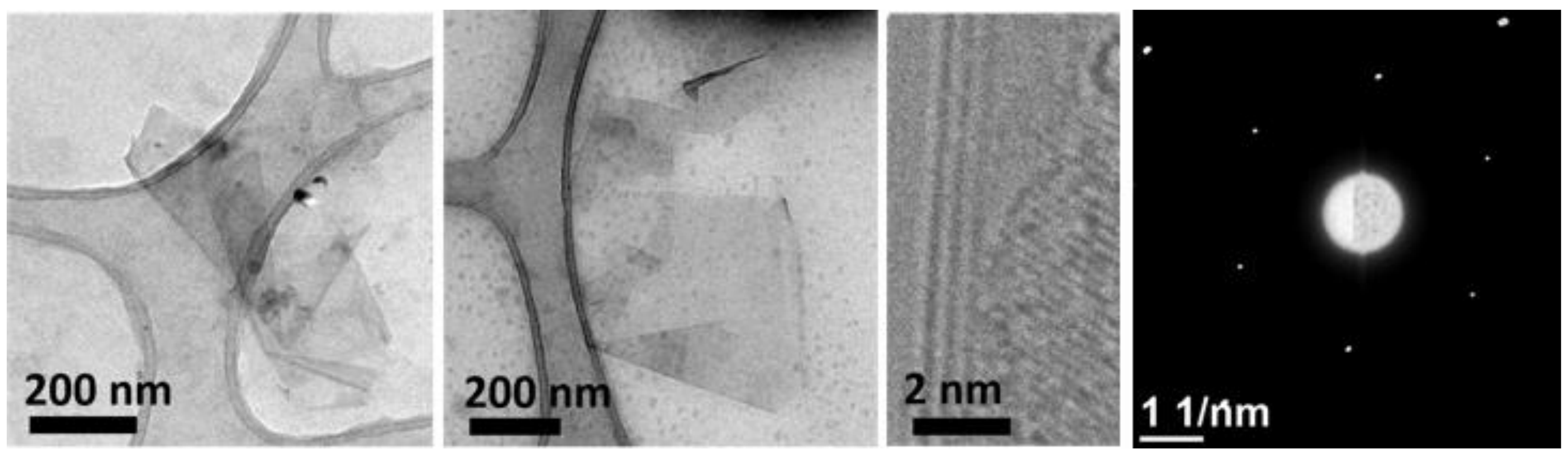
LPE of graphite → **Centrifugation** → **dispersibility**

Pristine graphite exfoliated in three PVA ($1.3x10^5$, $3.1\text{-}5.0x10^4$, $1.3\text{-}2.3x10^4$ g/mol) aqueous solution with different content in a sonic bath

As-obtained graphene/ PVA/ water mixture centrifuged at 1500 RMP for 90 min

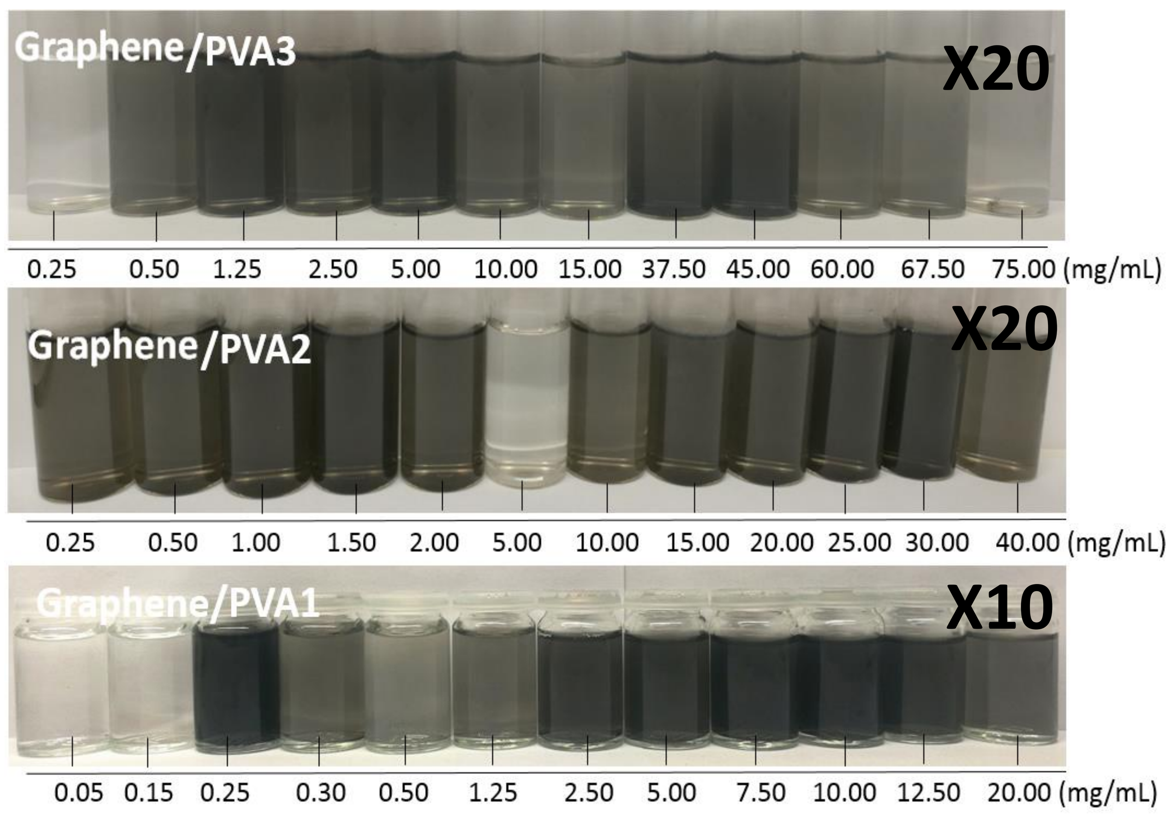
UV-vis absorption spectra used to evaluate graphene content.

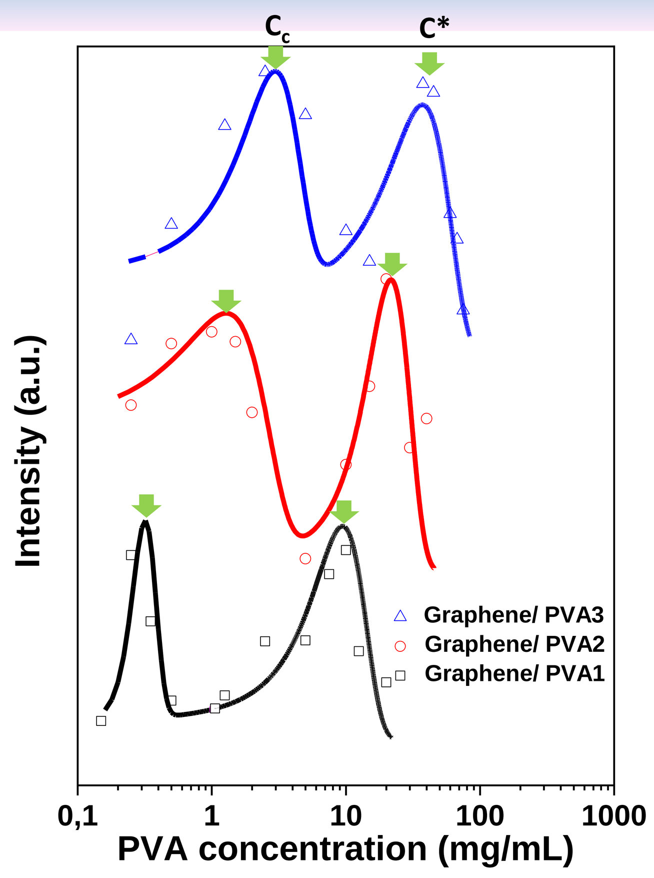
Characterization



TEM images of typical graphene in solution, and an electron diffraction pattern from a selected monolayer area at $Cp = 0.25$ mg/mL

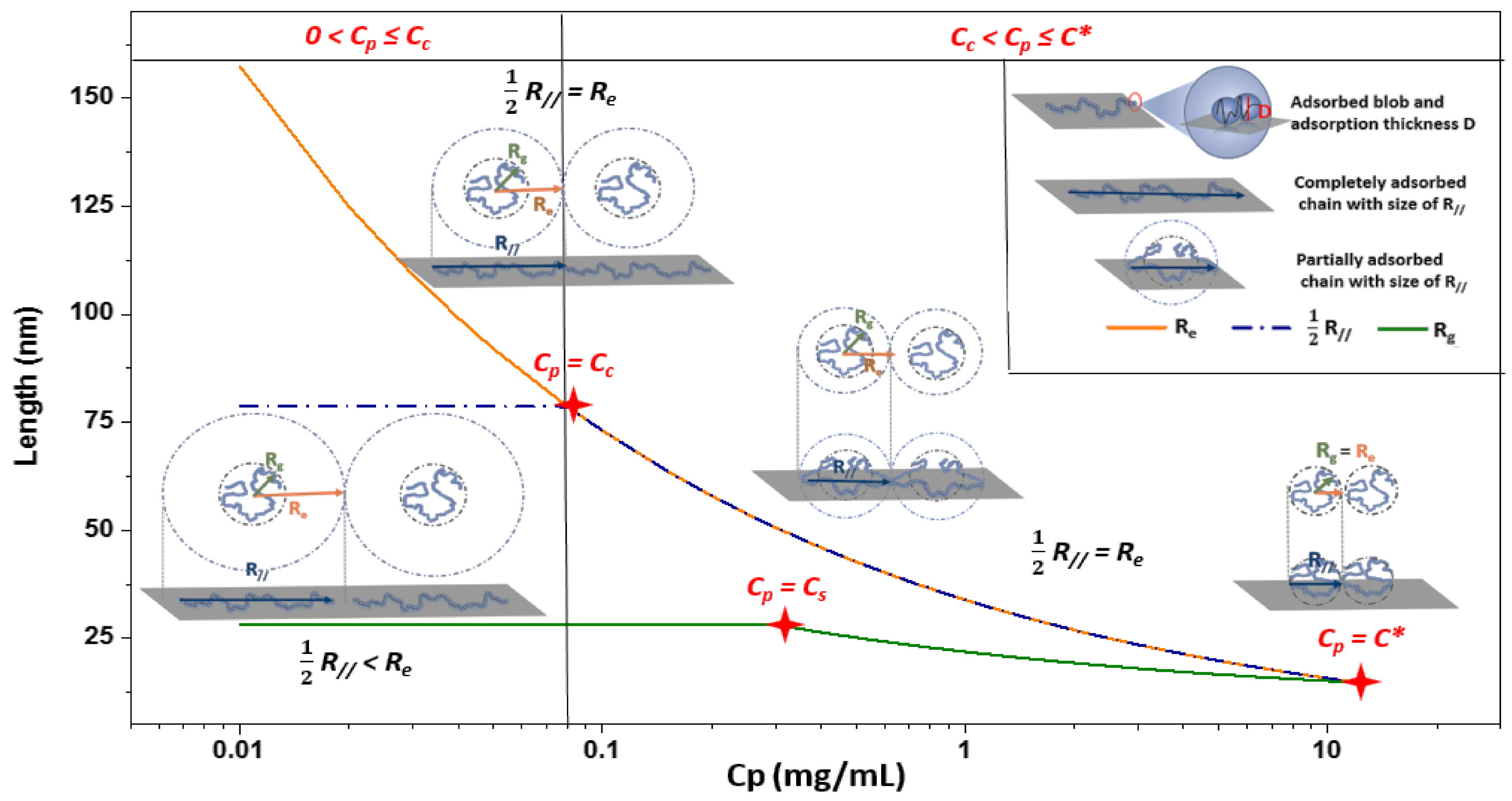
Result





Images of the graphene colloid in the PVA1, PVA2, and PVA3 solutions after dilution 10 (x10) and 20 times (x20). (**b**) UV-visible light absorption of graphene at λ = 660 nm curve *vs.* the PVA concentration

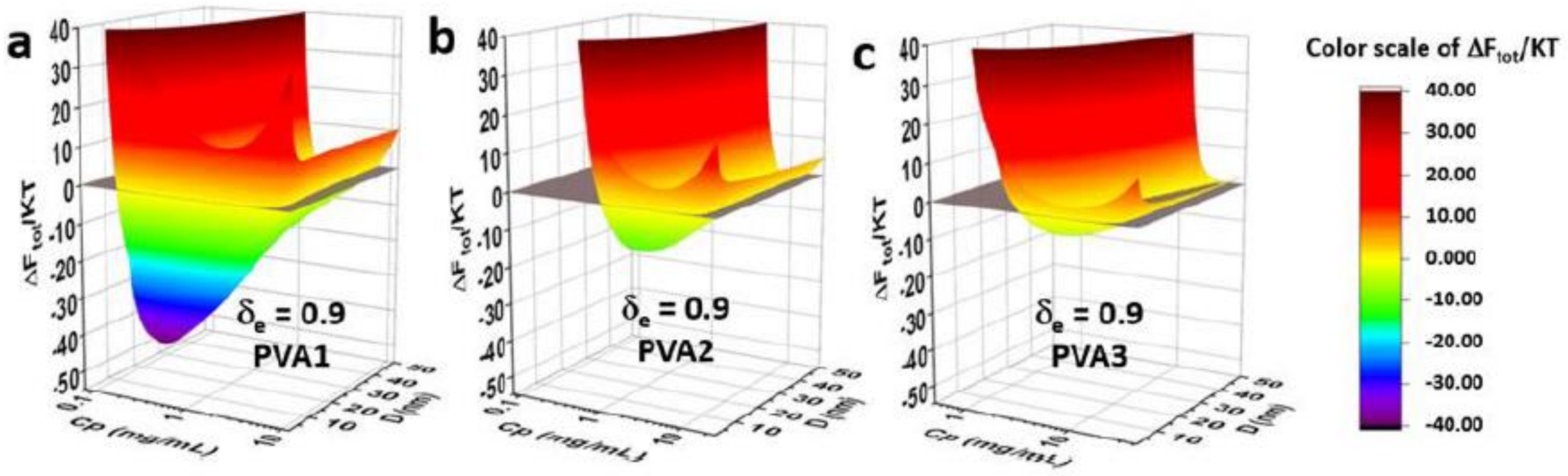
Adsorption model



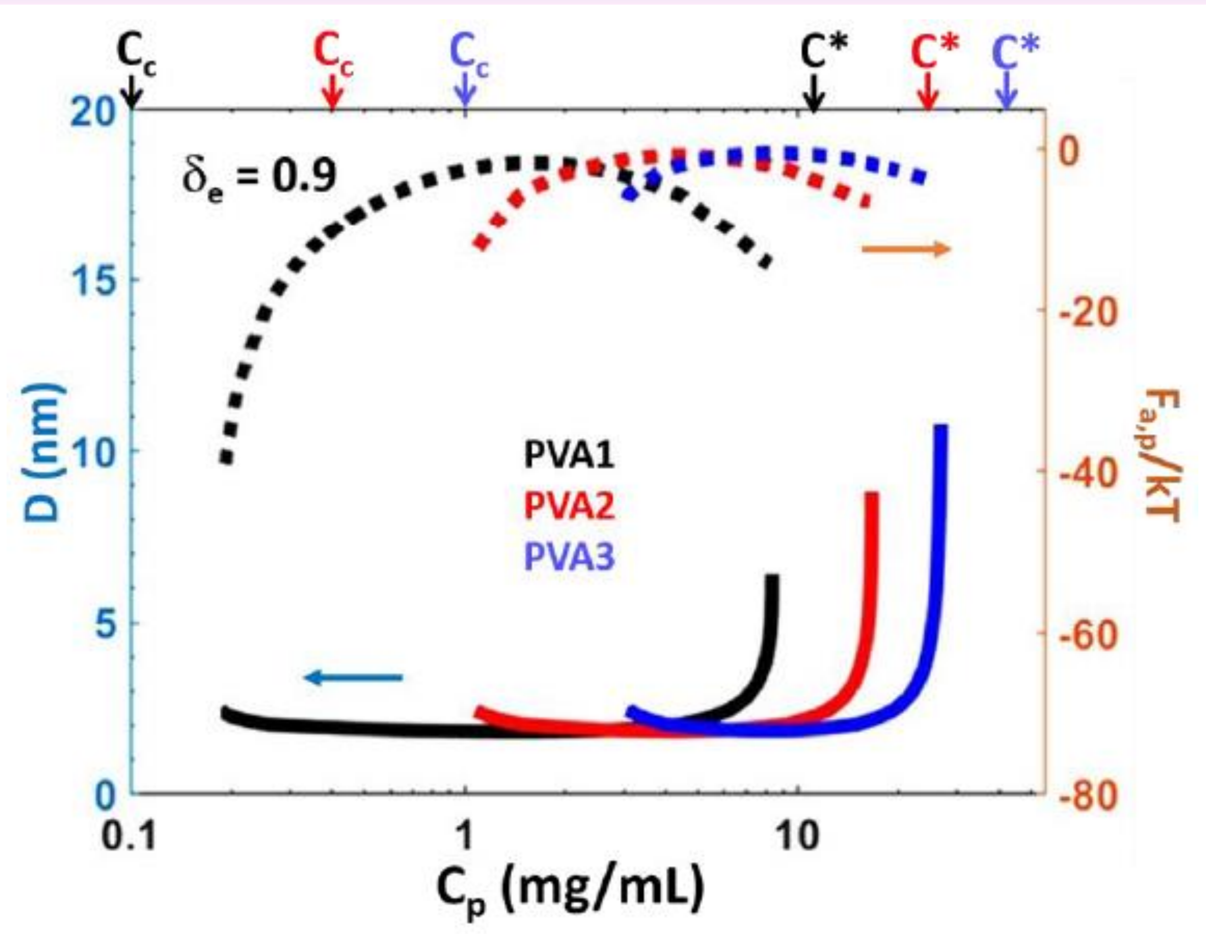
Adsorption process of polymer coils in "dilute" regime.

Mechanism

$$\Delta F_{tot} = F_{a,p} + F_{p,p} - F \approx \mathrm{k}TN^* \left[\left(\frac{b}{D}\right)^{5/3} - \delta_e \frac{b}{D} \right] + kT \left[\upsilon \frac{(N-N^*)^2}{R_{//}^3} + \frac{R_{//}^2}{(N-N^*)b^2} \right] - F \le 0$$



Calculated free energy ΔF_{tot} plotted as a function of the polymer concentration *Cp* (mg/mL) and adsorbed thickness *D* (nm).



Calculated adsorbed thickness *D* and free energy of adsorbed part $F_{a,p}$ in a partially adsorbed chain plotted as functions of the polymer concentration *Cp* when $\Delta F_{tot} = 0$.

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REFERENCES

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2. May, P., Khan, U., Hughes, J. M. & Coleman, J. N. *The Journal of Physical Chemistry C* **116**, 11393–11400 (2012).

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