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A REVIEW OF POLLUTANT'S INTERACTIONS ONTO CARBON NANOTUBES IN WASTEWATER TREATMENT USING DENSITY FUNCTIONAL THEORY

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Abstract:

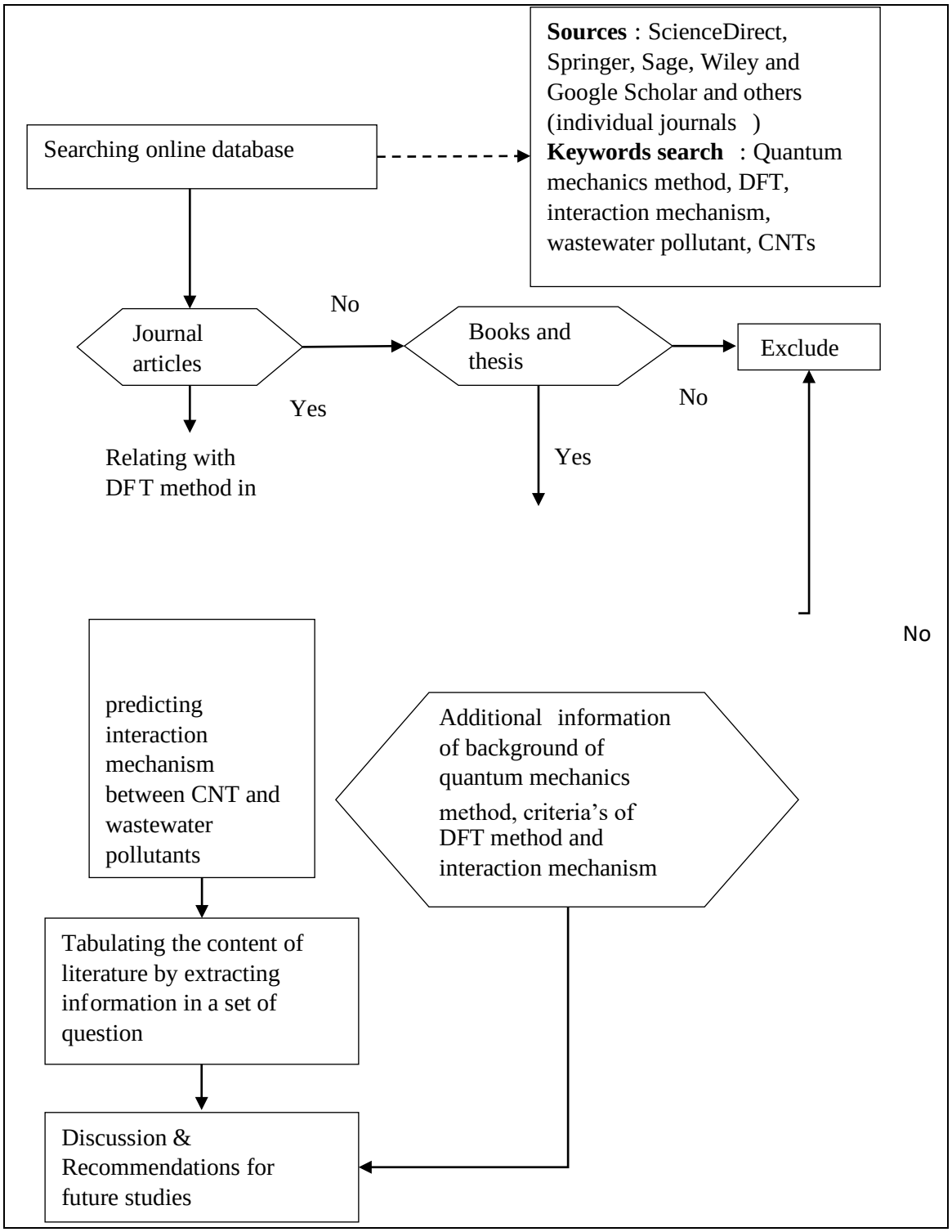
Due to the abrupt developments in industrialization and urbanization, various pollutants especially heavy metals and organic pollutants are largely found in the wastewater system. The removal of the pollutants in aqueous solution by using carbon nanotubes as adsorbent has become a popular topic in research studies. However, the theoretical study regarding on determination of the interaction mechanism between carbon nanotubes and wastewater pollutants have never been reviewed. In this study, a review of interactions between pollutants in wastewater and carbon nanotubes using density functional theory method are provided. Two significant methods have been carried out in the study. Firstly, the relevant literature from online database is collected and filtered by using the following keywords: "quantum mechanics method" OR "density functional theory (DFT)" OR "interaction mechanism" AND "carbon nanotubes (CNTs)" AND "pollutants". Secondly, the useful content in selected literature was tabulated by extracting information based on some research questions. Based on the findings, the wastewater pollutants that studied using DFT consist of heavy metals such as zinc (II), mercury (II), lead (II) and chromium (VI) and organic pollutants likes phenols, reactive blue dye, methylene blue, acridine orange dye and anthracene. Whereas, the carbon nanotubes found in the DFT studies are pristine SWCNTs and functionalized SWCNTs likes carboxylic functionalized CNTs and amidoamine functionalized CNTs. The common interaction mechanism found between the carbon nanotubes and organic pollutants are van der Waals interaction, electrostatic interaction, π- π interaction and hydrogen bond. Meanwhile, the interaction found between carbon nanotubes and heavy metal are electrostatic attraction, coordination bond and complexation interaction. The DFT method that are widely used is B3LYP method and split valence with diffusion and polarization basis set such as 6-31+G and 6-31++G (d.p). From the findings, the DFT computational method is proven to be a great tool in providing the insight of the nature of the adsorption of wastewater pollutants onto carbon nanotubes.

***Keywords*:**

DFT; Quantum mechanics; Interaction mechanism; Carbon nanotubes; Wastewater pollutants ***Objectives:***

- To summarize the differences of density functional theory (DFT) method in different wastewater system.
- To describe the mechanism of interactions of pollutants in wastewater onto carbon nanotubes (CNTs) surface using DFT method.

Methodology:



Results:

Wastewater pollutants	Carbon Nanotubes	Interaction mechanism	Findings
Organic pollutants			
Phenols	Pristine SWCNTs	Electrostatic interaction	[i]E_b = -34.19 kJ/mol [ii]D_b = 2.973 Å
Phenols	Hydroxyl functionalized CNTs (CNT-OH)	Hydrogen bonding and π- π interaction	E_b = -47.96 kJ/mol D_b = 2.704 Å
Reactive blue dye	SWCNTs	Electrostatic interaction	E_b = -75.26 kJ/mol D_b = 2.95 Å
Anthracene	SWCNTs	π- π interaction	E_b = -48.24 kJ/mol D_b = 3.10 Å
Acridine orange dye	SWCNTs	π- π interaction	E_b = -63.68 kJ/mol D_b = 2.54 Å
Methylene blue	SWCNTS	π- π interaction, electrostatic interaction	E_b = -99.38 kJ/mol D_b = 1.85 Å
Heavy metals			
Mercury (II)	Amidoamine functionalized CNTs	Complexation	E_b = -200 kJ/mol $D_{b\ (Hg\text{-}O)}$ = 3.792 Å $D_{b\ (Hg\text{-}N)}$ = 6.159 Å
Zinc (II) and Lead (II)	Nitrogen functionalized CNTs (CNT-ttpy)	Coordination bond	$E_{b\ (Zn)}$=-192.08 kJ/mol $E_{b\ (Pb)}$=-235.46 kJ/mol
Zinc (II) and Lead (II)	Carboxyl functionalized CNTs (CNT-COOH)	Electrostatic interaction	$E_{b\ (Zn)}$= -16.58 kJ/mol $E_{b\ (Pb)}$= -34.86 kJ/mol
Chromium	Titanium complexes SWCNTs	Chemisorption	E_b = -192.97 kJ/mol D_b = 1.90 Å

[i] E_b = Energy binding (kJ/mol)

[ii] D_b = Binding distance (Å) or closest distance between atom at carbon nanotubes and pollutants

Conclusion:

This review has covered the application of DFT method to elucidate the interaction mechanism between carbon nanotubes and pollutants in aqueous solution. The criteria of DFT method which consist of basis set, exchange correlation functional and solvent effect is investigated and shows different type of DFT method have been used for different wastewater system. The most popular DFT method in providing good approximation of geometrical structure are B3LYP method and split valance polarization basis set. Based on the review of past literature, the common interaction mechanism between CNTs and organic pollutants are electrostatic interactions, π-π stacking interactions and hydrogen bonding interaction. Whereas, heavy metals ion is adsorbed onto CNT surface through strong interaction energy such as coordination bond and complexation interaction. In summary, DFT method is convinced to be a useful tool in investigating the nature of nanoscale structure including properties of carbon nanotubes and the mechanism of pollutants uptake by the CNTs and the contents of this review is believed to be useful to researchers and practitioners that interested in the field.

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