Computational Insights into UV Spectrophotometric Behavior of PMMA in the Presence of Pharmaceutical Pollutants through Atomistic Calculations

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INTRODUCTION

Polymers are widely used in environmental applications, particularly in water treatment systems. Pharmaceuticals such as β-blockers (nadolol - NAD and pindolol - PIN) are emerging contaminants commonly found in water, posing significant risks due to their persistence and bioactivity. Understanding how these pharmaceuticals interact with polymers at the molecular level is crucial for optimizing their use in filtration and purification technologies. This work presents a computational study on how the adsorption of NAD and PIN onto polymethyl methacrylate (PMMA) affects the polymer's UV spectrophotometric properties. Using density functional theory (DFT) and simplified time-dependent DFT (sTD-DFT), we simulated the UV absorption spectra of PMMA before and after pharmaceutical adsorption. We aim to provide insights into the changes in PMMA's electronic structure resulting from these interactions.

COMPUTATIONAL DETAILS

METHODS

Geometric pre-optimization: GFN2-xTB method
Geometric optimization: r2SCAN-3c method
SPE calculations: M06-2X/6-311++G(d,p)
Excitations: sTD-DFT, ωB97X-D3/6-31G(d,p)
Solvation models: CPCM and ALPB

CODES

Semiepiric: xtb 6.7.1 (via atomistica.online platform)
DFT: ORCA 6.0
RDG: Multiwfn (via atomistica.online platform)

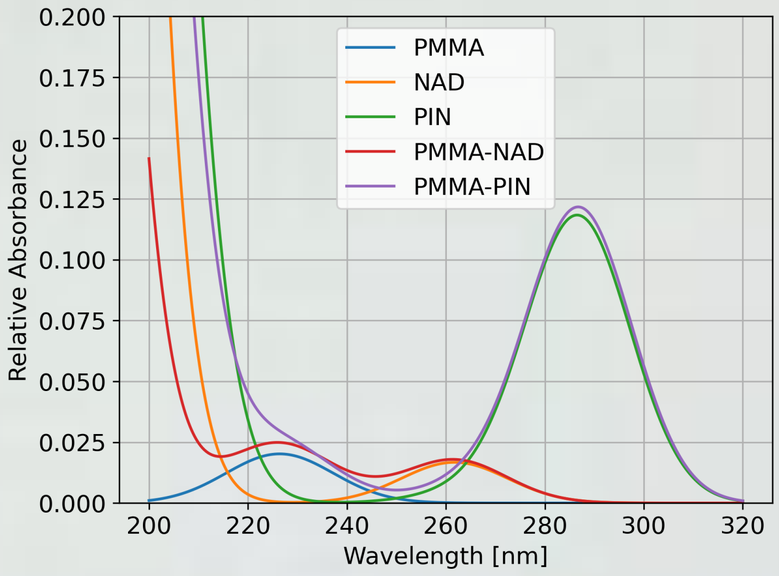

Figure 1. UV absorption spectra of PMMA, NAD, PIN and after adsorption of pharmaceuticals on PMMA.

RESULTS AND DISCUSSION

The UV absorption spectra of PMMA after pharmaceutical adsorption (Figure 1) shows slight changes in peak positions and intensities. These shifts suggest that the electronic environment of PMMA is altered by the presence of adsorbed NAD and PIN, primarily through non-covalent interactions. Intramolecular noncovalent interactions were addressed via the reduced density gradient (RDG) approach (Figure 2). The RDG scatter plot indicates that a greater number of attractive noncovalent interactions are formed during the adsorption of PIN by PMMA. On the other hand, RDG surfaces show that the attractive noncovalent interactions in the case of the PMMA-NAD interaction occur in the near vicinity of oxygen atoms close to the benzene rings of NAD, whereas in the PMMA-PIN interaction, they are concentrated around the nitrogen atom of the five-membered ring.

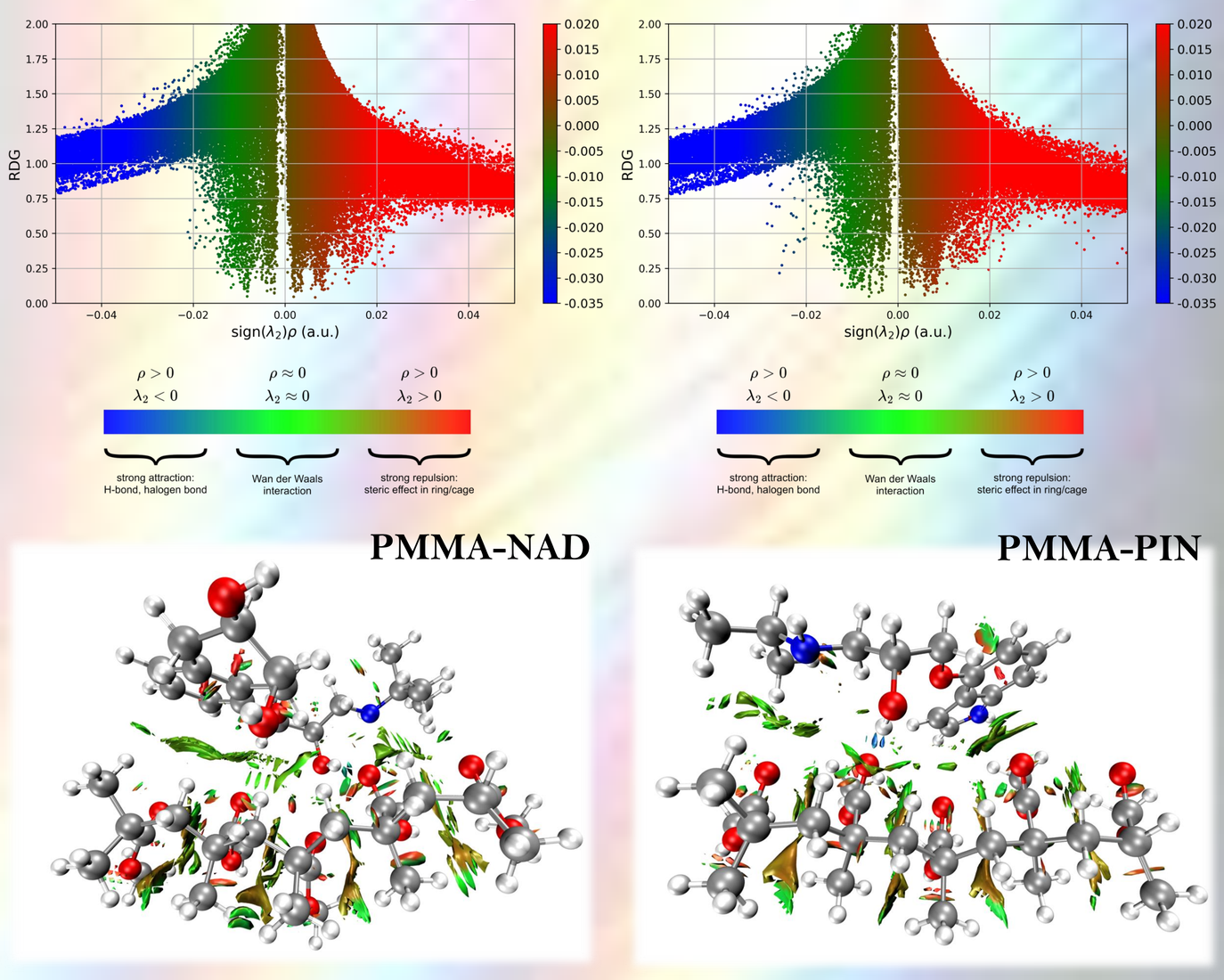

Figure 2. RDG scatter plots and RDG surfaces of PMMA-NAD and PMMA-PIN.

CONCLUSION

The computational approach provides a detailed understanding of interaction between molecules, which could aid in the design of advanced PMMA-based materials for the removal of pharmaceuticals from water. This study highlights the power of computational simulations in predicting UV spectrophotometric changes in polymer systems, contributing to the development of more efficient and environmentally sustainable water purification technologies.

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