Title: Insights into the adsorption performance of temozolomide on T-based 2D nanosheets from DFT and COSMO calculations

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Abstract: In this study, density functional theory (DFT) was employed to investigate the adsorption behavior and electronic interaction characteristics of the anticancer drug temozolomide (TMZ) towards T-graphene (T-G), T-boron nitride (T-BN), T-aluminum nitride (T-AlN), and T-gallium nitride (T-GaN). The primary objective of this study was to determine the most efficient nanocarriers for TMZ delivery. Several parameters were calculated, such as the adsorption energy, desorption time, dipole moment, electronic properties and quantum molecular descriptors, under both gas phase and aqueous conditions. The results demonstrated that the S1 configuration, in which TMZ is parallel to the nanosheets, provided the most favorable and stable interaction between TMZ and the nanosheets. Among the materials studied, the adsorption energy of T-AlN was strongest, at −1.56 eV. T-GaN also displayed favorable adsorption performance, with an adsorption energy of −1.16 eV. The HOMO–LUMO band gap reduced by 70.48% for T-AlN and 48.70% for T-GaN. These changes imply improved electronic conductivity and chemical reactivity. These properties are crucial for drug delivery. Furthermore, COSMO surface analysis revealed increased polarity and enhanced solubility of the drug-carrier complexes in aqueous media. This study suggests that T-AlN and T-GaN nanosheets could be suitable carriers for the anticancer drug TMZ.

Keywords:

https://pubs.rsc.org/na/article/8/8/2713/1229310/Insights-into-the-adsorption-performance-of