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Miscibility study of poly(ethylene glycol)-graphene oxide nanocomposites with ivermectin as potential drug delivery systems

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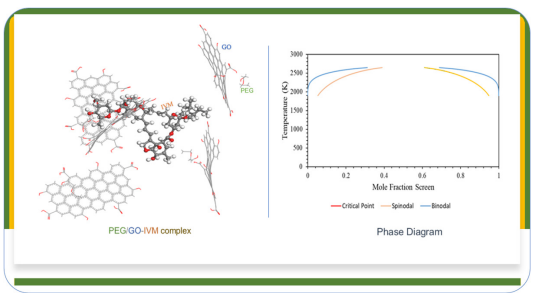
The interaction and the thermodynamic behavior of the carrier with the drug play a critical role in the development of a new drug delivery system. In this work, the miscibility of poly(ethylene glycol)-graphene oxide (PEG/GO) nanocarrier with ivermectin (IVM) in both gas and solvent media was examined using classical simulation. As such, binding energy distribution, phase diagram which shows the critical points, binodal and spinodal curves, the free energy of mixing isotherms, interaction parameter, χ and the distribution of Chi parameter with temperature were determined. In the gaseous state, the value of the interaction parameter, χ, is 102.93, and the energy of mixing is 60.95. Meanwhile, in a solvent medium, the value of the interaction parameter, χ and the energy of mixing are 85.31 and 50.52, respectively. These values suggest the disfavors of a mixed state for the excipient-drug system and an exothermic interaction, which means that the carrier will not interact to form a single phase with the drug. Consequently, the interaction of the molecules led to the development of two phases as shown by the presence of the binodal phase in the phase diagram. This outcome is further validated by the binding energy distribution curve. Therefore, the immiscible nature of the carrier and the drug, suggests that PEG/GO nanocomposite can serve as a potential nano vehicle for the delivery of IVM without leading to the formation of a miscible complex.

Graphical abstract



Recent Publications

1. Adekoya, O. C.; Adekoya, G. J.; Sadiku, E. R.; Hamam, Y.; Ray, S. S., DFT Interaction Study of Polyethylene Glycol-Based Nanocomposite with Cephalexin Drug for the Elimination of Wound Infection. ACS Omega 2022, 7, 38, 33808–33820. https://doi.org/10.1021/acsomega.2c02347

2. Adekoya, O.C.; Adekoya, G.J.; Sadiku, E.R.; Hamam, Y.; Ray, S.S. Application of DFT Calculations in Designing Polymer-Based Drug Delivery Systems: An Overview. Pharmaceutics 2022, 14, 1972. https://doi.org/10.3390/pharmaceutics14091972

3. Adekoya, O. C.; Yibowei, M. E.; Adekoya, G. J.; Sadiku, E. R.; Hamam, Y.; Ray, S. S., A mini-review on the application of machine learning in polymer nanogels for drug delivery. Materials Today: Proceedings 2022, 62, S141-S144. https://doi.org/10.1016/j.matpr.2022.02.101

Biography

Oluwasegun C. Adekoya is currently a postgraduate student of both Prof. Sadiku E.R. and Prof. Ray and conducts his research at their respective laboratories. His master's degree research at the Department of Chemical, Metallurgical, and Materials Engineering, Tshwane University of Technology, is about the DFT interaction study of a polyethylene glycol-based nanocomposite with the cephalexin drug for the elimination of wound infection. He recently published his articles in MDPI Pharmaceutics and ACS Omega. He has worked at the Lagos University Teaching Hospital (LUTH), SGS Société Générale de Surveillance (SGS), University of Nigeria Teaching Hospital (UNTH), National Orthopedic Hospital Enugu (NOHE), Reddington Hospital, and Premier Specialist Medical Center (PSMC). His current research is geared towards the potency of functionalized biopolymer nanogel as a potential antiviral drug delivery strategy to combat the viral SARS-CoV-2 and its variants. Furthermore, his area of focus is molecular diagnostics, nanotechnology, and biopolymers for drug delivery.

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