Issue 30, 2025

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From the journal:
New Journal of Chemistry

Design and development of La(III) driven graphene oxide superabsorbent hydrogel from guar gum and gallic acid for drug delivery applications: experimental and DFT evaluation

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Abstract

The use of graphene oxide (GO) and La^{3+} ions to reinforce guar gum (GG) and gallic acid (GA)-based hydrogel beads offers a promising strategy for controlled drug delivery. Hydrogels were synthesized *via* the solvent rotation method and characterized using SEM, FTIR, texture analysis, and TGA. Also, the complex of GO, GG, GA and La^{3+} was optimized at the DFT level of theory using the Stuttgart–Dresden (SDD) basis set along with WB97XD as the functional to infer various physicochemical properties. The calculations show that the central ion plays an important role in the adsorption model revealing the critical role of La^{3+} in enhancing adsorption properties in relevance with the target study. GO incorporation improved the swelling behavior (up to 3500% at pH 7) and increased the compressive strength from 83.24 N to 91.25 N. The drug encapsulation efficiency for amoxicillin trihydrate (Amox) was 88.3% (with GO) and 88.7% (without GO). Drug release followed the Korsmeyer–Peppas model (R^2 ≈ 0.98), achieving 60% release at pH 7.4 over 6.5 hours. These findings highlight the potential of GO-reinforced hydrogels for efficient and pH-responsive drug delivery at the experimental and DFT convergence.