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Metronidazole Drug Delivery: Theoretical Investigation of the Intercalation in the Interlayer Clay

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Abstract—This article presents a theoretical study of the interactions of the drug Metronidazole (Mt) intercalated in interlaminar Montmorillonite (MMT), where the geometry optimization was done by the Forcite module of the Materials studios 7.0 software, modifying the cations (Ca^{2+} , Mg^{2+} , Na^+ , K^+ , Fe^{3+} , Li^+) of MMT. The results obtained after the geometrical optimization of Mt in MMT are differentiated according to the type and nature of intercalation cations and the number of MMT layers. This article also shows that montmorillonite is a good way to test or improve the dissolution of the drug, but taking into account the nature, such as the type of cation used in montmorillonite and the number of layers of clay. According to our study, we can choose the best cation of clay that meets our interests and determines our strategy of working in the field of clays and drugs. The exothermic reactions are predicted by the interactions between the drug molecules and each cation and by the electrostatic force created between the layers.

Keywords: Electrostatic force; Montmorillonite; molecular simulation; intercalation in Montmorillonite; interlayer cation.