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Understanding the influence of pH/pKa by theoretical and computational method for loading/release of Ibuprofen

In this study, we present a theoretical model that combines with quantum mechanical calculation theory and pKa to anticipate the degree of interaction between acid-/base –dependent species over a full range of pH conditions. To validate the theoretical model, we have the drug loading and release of a pH-responsive drug delivery system consisting of Ibuprofen an anionic Non-steroidal anti-inflammatory drug molecule, functionalized with trimethylsilyl (TMS) mesoporous silica surface. The model relies on the possible combinations of pH-dependent states of the surface (S) and drug (D) molecules as neutral (0) and deprotonated (−1) states, whose relative probabilities depend on their pKa value and the desired pH. The four possible combinations were identified as S0D0, S0D−1, S−1D0, and S−1D−1, and periodic density functional theory calculations were performed for systems comprising drug fragments adsorbed onto a model TMS-functionalized quartz surface to calculate the pH-dependent interaction energy (E_pH^int pH). The E_pH^int value showed that the drug was loading in an acidic environment of stomach (pH 2–5), and releasing at neutral or slightly basic pH in the small intestine (7.4);
the behavior is in accordance with the experimentally reported date.

Presenter Biography

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