Predicting Particle Properties of Organic Materials using Surface Descriptors

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Particle properties are responsible for a large number of manufacturing and product performance issues within the formulated product industries, such as fast-moving consumer goods, pharmaceuticals, agrochemicals, and dyes [1]. The surface chemistry and roughness of particulates can influence processing qualities such as flow, hygroscopicity, packing, and sticking. Understanding these particle properties plays a crucial role in formulation decisions and typically requires extensive trial and error studies with a high material cost. Computational tools for predicting surfaces have been extensively utilised to visualise the positions of chemical groups and postulate possible interactions based on steric hindrance or energy calculations[2]. These are either qualitative or time-consuming to calculate.

We present an accessible method for quantifiably predicting particle properties using a single crystal structure and demonstrate the use of interaction data from the Cambridge Structural Database (CSD) to predict possible surface interactions [3]. Here we assess how Ibuprofen's predicted particle properties correlate with the punch-sticking properties reported by Hooper et al. [2]. Their study found ibuprofen exhibited different punch-sticking behaviour depending on the particle morphology, and they attributed the difference in particle properties to the surface chemistry. We present an extension of their work and quantifiably describe the differences for the given morphologies using experimentally determined shapes [2,4].

We identify the most electrostatic and polar surfaces using chemical surface descriptors and surface charges. The roughness of each facet is quantitatively described and compared to understand its role in the final particle performance. Each morphology facet was surveyed for possible surface interactions using a range of electronegative probes to understand how the particles would interact with the tablet press. This methodology allows for rapid qualitative and quantitative analysis aiding formulators and particle designers in making informed, data-driven decisions to help de-risk their formulations.

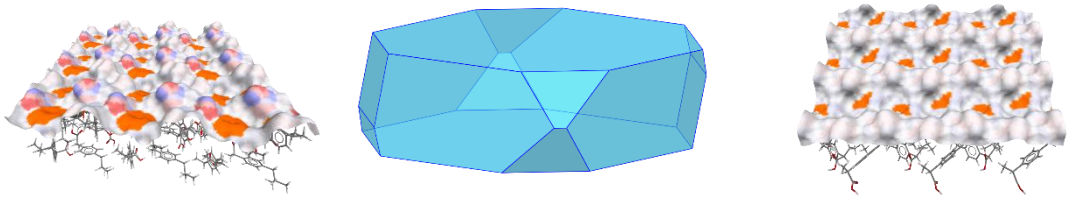

Figure 1 - Morphology of ibuprofen and two surfaces displaying surface charge (red/blue) and aromatic bonds (orange).

References

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