"Particle Informatics": Evolving methods for understanding particle properties

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In recent years, considerable investment has been made towards advancing pharmaceutical development and manufacturing through Digital Design approaches [1]. Industrial scientists are moving away from time and resource intensive screening techniques to more rapid *in silico* methods to inform key decisions throughout the drug manufacturing process.

The links between solid form and structural properties are well developed [2], but our understanding of the relationship between particle and surface properties and downstream manufacturability of an Active Pharmaceutical Ingredient (API) are considerably less established. By providing new methods for visualising and describing these key attributes, we can gain a deeper insight into properties that contribute to the way particles flow or how they form tablets under compression.

Since describing these approaches and their application to the drug lamotrigine [3], we have continued to develop and refine the way that we can describe a particle and its properties. This presentation will discuss those advances and the challenges that lie ahead.

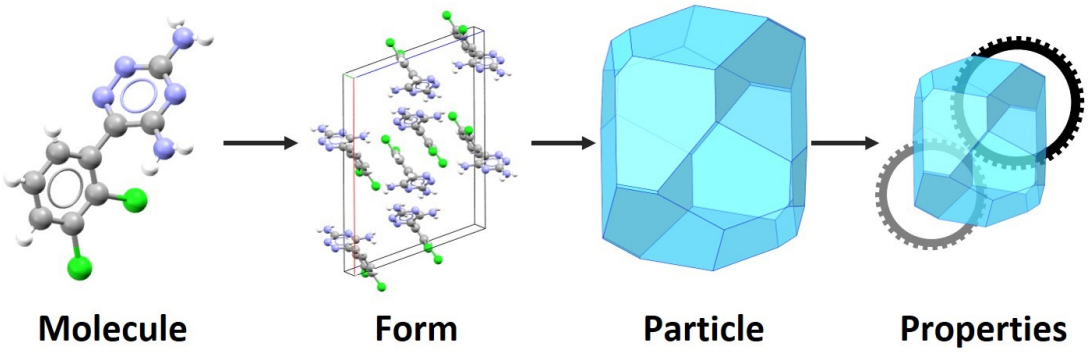

Figure 1. The "Particle Informatics" workflow follows the journey from molecule to product.

[1] www.addopt.org

[2] Galek, P. T. A., Pidcock, E., Wood, P. A., Bruno, I. J. & Groom, C. R. (2012). *CrystEngComm*, **14**, 2391-2403.

[3] Bryant, M. J., Rosbottom, I., Bruno, I. J., Docherty, R., Edge, C. M., Hammond, R. B., Peeling, R., Pickering, J., Roberts, K. J. & Maloney, A. G. P. (2019). *Cryst. Growth Des.* **19**, 9, 5258-5288.

Keywords: pharmaceuticals; digital design; particle properties; structure property relationships