Physical Chemistry Seminar

Wednesday, January 17, 2018

12:30 pm, BRWN 4102

COMPUTATIONAL SOLID-STATE CHEMISTRY APPLICATIONS IN PHARMACEUTICAL INDUSTRY

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Given the complexity of the pharmaceutical solid-state landscape and challenges facing the pharmaceutical industry, an accelerated Drug Development greatly benefits from guidance provided by computational methods. The emerging field of Computational Pharmaceutical Solid State Chemistry covers the whole spectrum of state-of-the-art computational approaches, which are used to support all steps related to the development of solid-state pharmaceuticals.[1]

This presentation will focus on computational support of such important tasks as decrease of pharmaceutical crystals agglomeration; impurity purge *via* recrystallization; coformer selection for cocrystallization and improved stability at a high relative humidity; and solid form selection.

1. Abramov, Y.A., Ed. *Computational Pharmaceutical Solid State Chemistry*, John Wiley & Sons, 2016.