Editorial

As this is the first issue in 2021, on behalf of the whole team of the journal *Powder Diffraction*, I would like to wish all our readers, authors, and team members happiness, health, and continued scientific accomplishments in 2021. I hope also that as we work through 2021 that with vaccinations and continued safe practices the COVID-19 virus comes under control and hopefully all may steadily return to pre COVID-19 levels of scientific discovery and communication.

A large fraction of the manuscripts in this issue of *Powder Diffraction* (PDJ) are related to pharmaceutical compounds and their exceptional characterization by structure solution, Rietveld analysis, and density functional theory (DFT) energy minimization. Two aspects are noteworthy. First, the growing emphasis on the number of PXRD manuscripts related to the characterization of pharmaceutical materials likely corresponds to the growth of the importance of pharmaceutical materials in society. Second, each of the published manuscripts used various codes for structure solution and Rietveld analysis for the determination of a structural model followed by structural and packing energy minimization using DFT. Quite often, the two refinement methods are in excellent agreement regarding the "best" model for the crystal structure.

The use of PXRD indexing, structure solution, and Rietveld analysis has been a mainstay of powder diffraction structure analysis for many decades. During this time, the software tools available have significantly improved and today, with quality PXRD data, can be quite powerful. However, in recent years, PXRD structural analysis has been complimented with the use of DFT techniques that further optimize the structure by minimizing the packing energy of the crystalline structure. The growth of the manuscripts using all three of these techniques submitted to *Powder Diffraction* has been significant and, in this issue, reached a particularly high level of over 90%!

Clearly, the trend line of what constitutes a state-of-the-art analysis of a structure solution for organic crystalline pharmaceutical materials is expanding. Adding DFT energy minimization to further optimize the structural model and aiding in understanding the hydrogen bonding and other crystal packing forces is becoming the future for organic crystal structure analysis.

As you read the manuscripts in this issue of PDJ consider if you should adopt the DFT computational sophisticated tools as part of your organic structural analysis.

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