Poster Presentation

MS112.P06

Theoretical Prediction of Crystal Polymorphs for Organic Molecules

S. Obata[1], M. Sato[2], H. Goto[2]

[1]Toyohashi University of Technology, Promotion Office of Advanced Simulation Engineering, Toyohashi, Japan, [2]Toyohashi University of Technology, Department of Computer Science and Engineering, Toyohashi, Japan

Crystal structure prediction is one of the useful theoretical tools for designing and synthesizing new materials in pharmaceutical therapeutics and industrial electronics. Furthermore, the prediction can provide immense valuable scientific knowledge on a crystal growth, polymorphism and many properties of organic molecular crystals. Therefore, we have started the development of high-speed and high-accurate prediction method for organic molecular crystal structures [1,2]. In this work, we demonstrate the theoretical predictions of crystal structures of fourteen target molecules that were used in the international competitions known as CSP blind tests hosted by CCDC [3]. All strategies required for crystal lattice construction expanded to a given effective crystal radius, crystal energy calculation with the reliable molecular force field (MMFF94s) and exhaustive geometry search included a variety of crystal polymorphism are implemented into CONFLEX program [1]. As the results of the applications, we confirmed in all cases of target molecules that, at least, one calculated crystal structure in agreement with the corresponding observed ones can be found. Essential ability required for the prediction method to survive the CSP competitions is that the experimental crystal structure can computationally reproduce within top 3 of most stable structures in crystal energy evaluation. In these tests, only three applications to the target I (Orth. polymorph), II and VIII can successfully satisfy the demand. Details will be discussed in this conference.

[1] *H. Goto, S. Obata, N. Nakayama, K. Ohta, CONFLEX7; Conflex: Tokyo, Japan, 2012.,* ***[2]*** *S. Obata, T. Miura, Y. Shimoi, Jpn. J. Appl. Phys., 2014, 53, 01AD02.,* ***[3]*** *D. A. Bardwell et al, Acta Cryst. Sec. B, 2011, 67, 535-551.*

Keywords: crystal structure prediction, blind test, polymorphism