Simulating Nanostructures: 2D-periodic organic semiconductors

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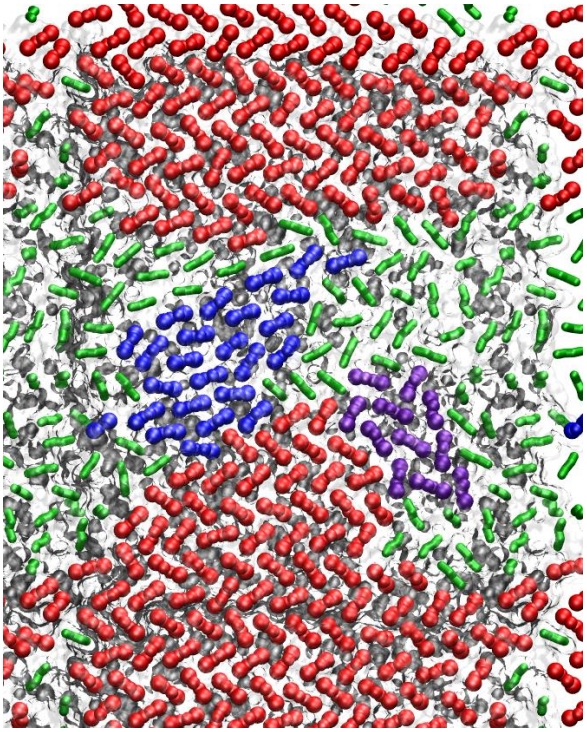
Organic semi-conductors surround us in daily life. Two years ago we have presented an n–type semiconductor system of C_{60}–C_{18}–PA.[1] Now we have simulated and analysed a p–type organic semi-conductor system of benzothieno[3,2—b][1]benzothiophene (BTBT) on an aluminum oxide surface. Special focus in this part of the work is the structure of organic molecules. Differences in structure between C_{11} and C_{12} BTBT have been worked out which agree with experimental results. In this talk we present results we have gained from molecular dynamic simulations we have performed on this 2D system.



(1) Jäger, C. M.; Schmaltz, T.; Novak, M.; Khassanov, A.; Vorobiev, A.; Hennemann, M.; Krause, A.; Dietrich, H.; Zahn, D.; Hirsch, A.; Halik, M.; Clark, T. *J. Am. Chem. Soc.* **2013**, *135*, 4893.