

## Poster Presentation

MS112.P01

### *Structure prediction of N-heteroacenes as potential organic semiconductors*

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Organic electronics offer exciting new alternatives to traditional inorganic devices based on advantages such as lower cost, ease of manufacture and flexibility. Small molecule semiconductors such as pentacene and rubrene are the focus of intense research due to performance approaching that of inorganic semiconductors. Charge transfer in polyaromatic hydrocarbons (PAHs) relies on the degree of  $\pi$ -conjugation and overlap of the  $\pi$ -systems of neighbouring molecules in the solid state. Small changes in the intermolecular interactions can lead to important changes in crystal packing and electronic properties. Thus, functionalization of PAHs is often used to improve their packing in the solid state. The addition of electronegative atoms into the ring system of pentacene has been proposed for improving stability while retaining attractive properties. [1] N-heteroacenes result from the substitution of nitrogen into the arene ring structure. The resulting potential for weak hydrogen bonding could direct coplanar molecular arrangements, sheet formation and favourable  $\pi$ -overlap for charge transport. Theoretical studies [2] have been carried out showing promising properties at the molecular level. As of yet no analysis of the solid state of these molecules has been performed to investigate how this substitution affects the packing and electronic properties. Here, we present the results of crystal structure prediction studies and calculation of charge transport properties aimed at understanding the influence of nitrogen substitution on the crystal packing of N-heteropentacenes and their performance as semiconducting materials.

[1] Bunz, U.; Engelhart, J.; Lindner, B.; Schaffroth, M., *Angew Chem. Int. Ed.* 2013, [2] Winkler, M.; Houk, K., *J. Am. Chem. Soc.* 2007, 129 (6), 1805-1815.

**Keywords:** Structure prediction, Organic semiconductors