Monte Carlo simulations of 2D molecular self-assembly

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Controlling the formation mechanism of organic thin films (OTFs) tailored by weak interactions on van der Waals (vdW) substrates provides an opportunity to obtain highly stable, large-area, and high-quality organic electronic devices [1]. To this end, understanding the self-assembly of organic molecules, like pentacene, from a disordered state into ordered 2D crystals is of great importance.

We use classical Monte Carlo simulations in order to study the growth of OTFs on monolayer substrates (graphene, hexagonal boron nitride). We investigate the intrinsic driving mechanisms responsible for the molecular ordering and analyze the role of the substrate for the growth process. In particular, we are address the question of controlling the orientation of the molecules. Further, we study the influence of temperature on the resulting aggregates. Our work complements a recent study based on molecular dynamics simulations [2].

Figure

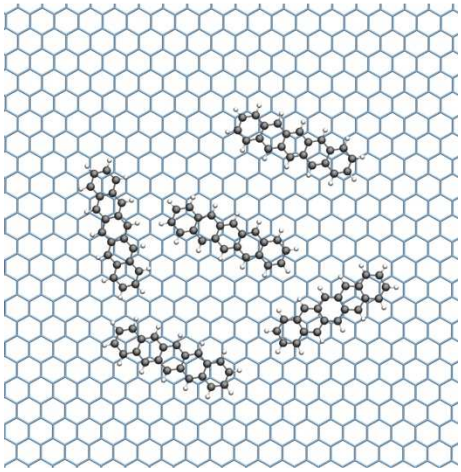

Figure 1. Intermediate step of the self-assembly process of pentacene molecules on a graphene substrate (schematic).

References

[1] Kumar et al, Nanotechnology **28**, 082001 (2017).

[2] Zhao et al, J. Phys. Chem. Lett. **6**, 4518 (2015).