How to image the structural details in molecular framework of the imine-based 2D polymers

Baokun Liang, Christopher Leist, Yingying Zhang, Zhiyong Wang, Renhao Dong, Thomas Heine, Xinliang Feng, Haoyuan Qi, Ute Kaiser
Electron Microscopy Group of Materials Science, Albert-Einstein-Allee 11, 89081 Ulm, Germany
Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, 01062 Dresden, Germany
baokun.liang@uni-ulm.de

Due to the high electron beam sensitivity of 2D polymers (2DPs), TEM imaging of their single molecular building blocks remains a challenging task. One crucial factor influencing the specimen stability is the acceleration voltage. Here we quantitatively analyzed the dependence between the acceleration voltage and the available structural information, similar to [1]. A systematic analysis of the 2DPs at the acceleration voltages of 80, 120, 200, and 300 kV was applied. Our results demonstrated that 120 kV is superior to the traditionally applied high acceleration voltages of 300 kV by approximately 5-7 % higher information gain.
By utilizing 120 kV and combined with low-dose technique, we have successfully imaged imine-based 2DPs with sub-2 Å resolution (see Fig. 1), which enables the direct observation of the structural details in the moleculer framework. The enhanced image contrast compared to imaging at 300 kV allowed for image acquisition with low defocus values, this greatly facilitates direct image interpretation and avoids confusion due to delocalization under high defocus, which is important for elucidating non-periodic features such as defects, grain boundaries, and pore interfaces. Thanks to this high image contrast, we have also obtained HRTEM images of glassy 2DP, for an efficient quantitative image analysis, a neuro-network was applied.

References

[1] Peet, M. J., Henderson, R. & Russo, C. J. , Ultramicroscopy, 203 (2019) 125–131 The energy dependence of contrast and damage in electron cryomicroscopy of biological molecules.

Figure

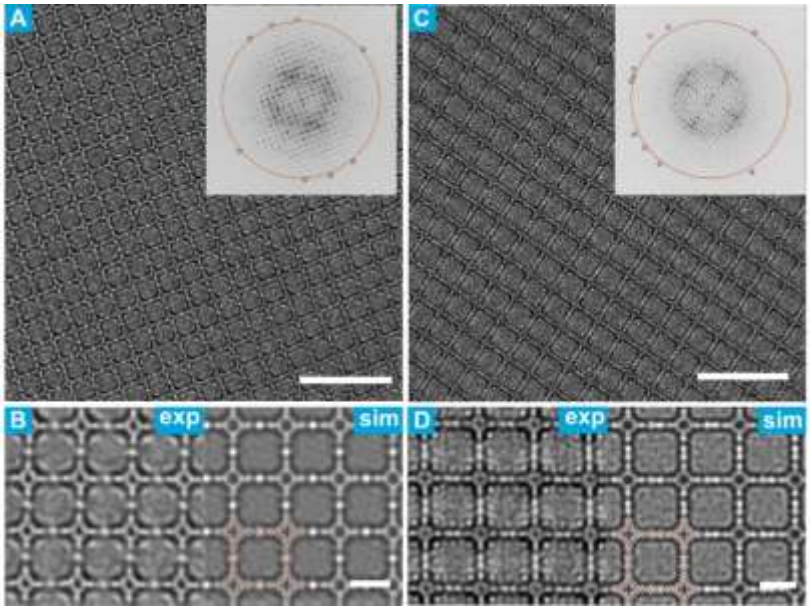

Figure 1: Experimental HRTEM images and simulations of 2D polyimine (PI) and biphenyldiyldimethanol (BPH). (A) shows the HRTEM image of 2D PI, scale bar: 10 nm. Inset: fast Fourier transform (FFT) patterns. The orange circle marks the spatial resolution of 2 Å. (B) includes enlarged experimental image and simulation result, scale bar: 2 nm. The atomic model is overlaid. (C) the HRTEM image of 2D BPH, scale bar: 10 nm. Inset: FFT patterns. The orange circle marks the spatial resolution of 2 Å. (D) enlarged experimental image and simulation, scale bar: 2 nm. The atomic model is overlaid. The DFT caculations were conducted for the atomic models.