Neural-network-based investigation of defect-rich carbon monolayers

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Defect-rich and amorphous 2D carbon monolayers are highly interesting in the grand family of 2D materials with potential applications in, e.g., DNA sequencing, catalysis. Since aberration-corrected high-resolution transmission electron microscopy (AC-HRTEM) allows for unambiguous elucidation of atomic structures down to sub-Angstrom scale, revealing the atomic structure of defect-rich and amorphous 2D can be achieved [1,2,3]. However, due to the lack of long-range order, quantitative description (e.g., degree of disorder, defect density and distribution) of such materials over large areas and sampleset sizes is still lacking. Conventional image analysis methods, e.g., handcrafted filter kernels, often require heavy user supervision and tremendous time cost, posing strong limitations on the data volume which can be realistically evaluated. The incompetence in handling big data volume also incurs the risk of user-induced selection bias, leading to overestimation of low-probability phenomena. Image analysis technique that could offer automation, precision, and extensive statistics, is thus highly desired. To reach this goal, convolutional neural networks [4] are employed. By determining the positions of every single atom in the AC-HRTEM images, the distribution and local variation of bond lengths and angles can be evaluated statistically and tracked through an image series. In addition, the neural network is capable of polygon mapping, providing not only the occurrence frequency of *n*-membered carbon rings but also their real-space distribution. A combination of networks can be applied to automatically evaluate image series, including automatic exclusion of image regions unusable for evaluation. This method results in large statistics thus reducing the impact of individual errors, such as, image artefacts or misinterpreted spots in an image. The networks are trained with simulated data, which reduces user bias and gives a time efficient way of generating the required training data.

References:

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[3] Toh, Chee-Tat, et al. "Synthesis and properties of free-standing monolayer amorphous carbon." *Nature* 577.7789 (2020): 199-203.
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Figures

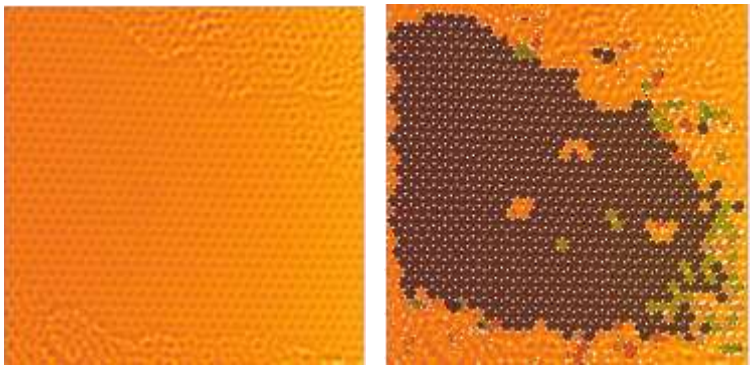

Figure 1: Left: AC-HRTEM image (false-colored) of CVD graphene acquired using SALVE microscope under 80 kV. Right: result after automatic evaluation. Atom positions marked in white, bonds between them in black, hexagons in brown, pentagons in orange and heptagons in green.