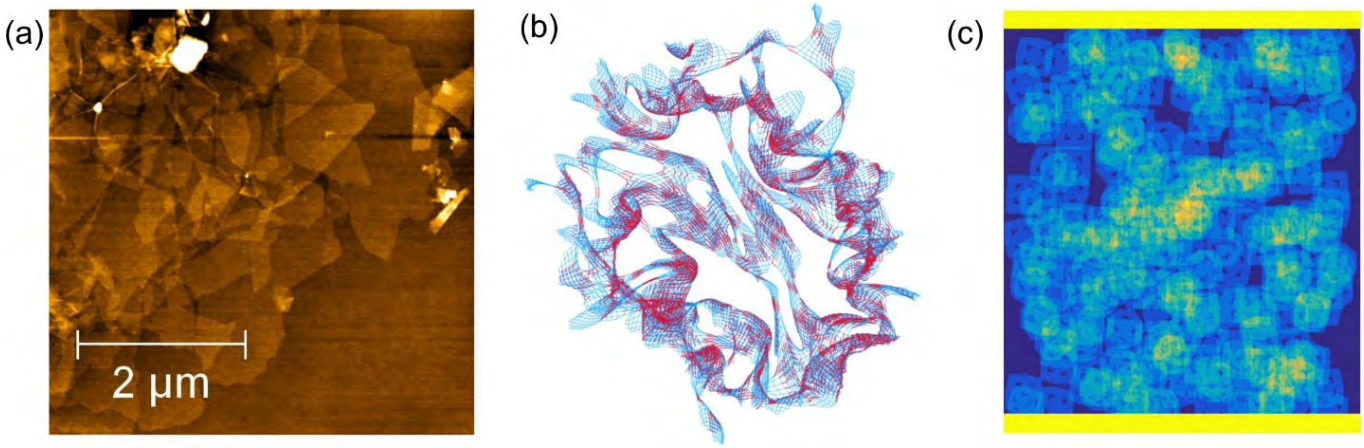
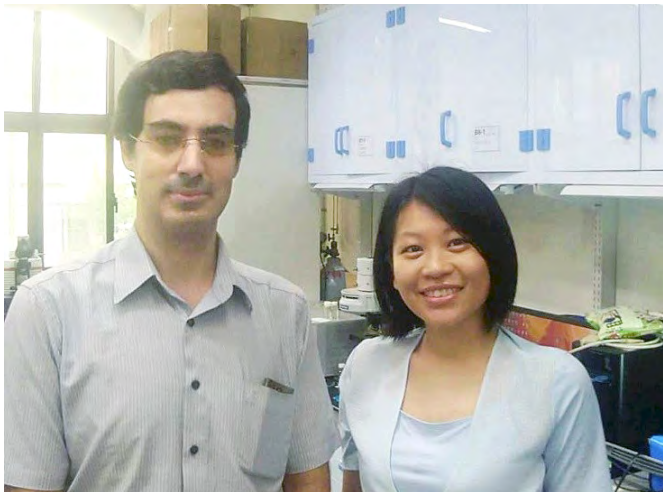
Emerging Simplicity from Complexity: A new Tool for Conduction in Nanostructure Assemblies

The last twenty years have seen a revolution of nanomaterials, such as nanotubes, flakes, and buckyballs, that are composed of only a few thousand atoms. To have an impact on our macroscopic world, millions of these nano-objects have to be combined. Such assemblies fundamentally change the properties of nanomaterials, which is both a challenge and opportunity for researchers. On the one hand, morphological degrees of freedom in materials introduce new sources of variabilities to materials synthesis. On the other hand, morphology-dependent properties represent new working principles for innovative sensors and energy generators. To support research in the production and application of nanostructures, a powerful modeling approach that considers complex morphology and diverse properties is required.

Prof. Ya-Ping Hsieh (Academia Sinica, Taipei, Taiwan) and Prof. Mario Hofmann (National Taiwan University, Taipei, Taiwan) published an article in *Nature Materials* describing a discretization approach that converts arbitrary nanostructures into a complex network of interconnected resistors and whose solution represents the spatial conductivity of nanostructure assemblies. This method is scalable to thousands of nanostructures and considers their internal conduction mechanism as well as the conduction between neighboring assembly constituents. In addition to being universally applicable to arbitrary nanostructures and assemblies, their approach can be implemented with simple and freely available tools that are accessible to researchers who have no prior experience in modeling.



A discretization approach models nanostructure films in (a) to a complex network of interconnected resistors depicted in (b), whose solution in (c) represents the spatial conductivity of nanostructure assemblies.



Using this new method, conduction could be calculated for the first time in realistic nanostructures, such as graphene flakes, polymer composites, and nanowires. Several emergent properties, such as sub-threshold percolation and percolation suppression, are predicted to be areas for future research.

An important application of the new capabilities is the extraction of important information on the single-nanostructure level from ensemble measurements. Culminating a decade of work by the researchers, experimental results on conduction in macroscopic nanotube films and graphene flake assemblies could be quantitatively reproduced by simulation. The results permit extrapolation toward the thickness and conductivity of a single flake or nanotube – parameters that have not been accessible to researchers before. The gained knowledge was employed to enhance the performance of graphene-based transparent conductors tenfold and identify its future suitability in such applications.

Finally, this approach could be used to predict potential candidates for future electronics. For this purpose, the performance of hundreds of nanostructure geometries and materials were characterized and new promising constituent geometries were observed.

In comparison to traditional methods and materials, this work paves the way for closer integration of materials modeling and experiments due to the new design freedom of nanostructure assemblies.

References

[1] Yao, H., Hsieh, Y., Kong, J., Hofmann, M., Modelling electrical conduction in nanostructure assemblies through complex networks. Nat. Mater. (2020). https://doi.org/10.1038/s41563-020-0664-1