

## Towards controlled growth of lowdimensional organic semiconductors on substrates: a theoretical understanding of their interaction mechanisms



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Organic semiconductors are promising candidates for a next generation of electronic devices; they offer a variety of new intriguing electronic phenomena while being environmentally friendly, inexpensive to produce, and mechanically flexible. Their mechanical flexibility enables them to be grown in various substrates, while their properties as well as morphologies can be greatly altered by the substrates. However, it is still a grand challenge to understand their interactions with substrates on a microscopic level and also to precisely control their morphologies. Organic-based molecular systems form various types of interfaces in zero to two dimensions, such as molecule-molecule interfaces and molecule-substrate interfaces. While understanding the fundamental nature of such interactions is a first key step in the path towards controlled growth of low-dimensional organic semiconductors, a precise and efficient description of their interactions is a theoretical challenge. In this talk I will discuss a couple of examples demonstrating the role of substrates in controlling the overall configurations of nanoscale organic semiconductors, nanowires, nanoislands and chains, and finally films. Different types of substrates such as semiconductor, insulator, and metals have significantly different types of atomic interactions, resulting in very distinctive semiconductor morphologies.

Mina Yoon received her Ph.D. degree in Theoretical Condensed Matter Physics in 2004, from Michigan State University, she joined ORNL as a postdoctoral researcher and a year later became Research Assistant Professor at the Physics and Astronomy Department of the University of Tennessee, Knoxville. From 2008-2011, she was awarded a Max Planck Fellowship. Since 2009, she is a Research Scientist at ORNL. The primary focus of Dr. Yoon's research lies in the fundamental understanding of growth mechanisms, novel properties, functionalization, and potential technological applications of surface- based and low-dimensional organic/inorganic hybrid materials. Especially, her interest is in utilizing these materials as light, environmentally friendly, and efficient energy storage/generation and optoelectronic application by making use of their unique low-dimensional properties. Her theoretical approach ranges from atomistic modeling by first-principles quantum mechanical approaches and many-body potential approaches, to continuum elasticity theory and phenomenological modeling. http://cnms.ornl.gov/contact\_us/YOON\_Mina.pdf

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