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Predictive Modelling of Supramolecular Assemblies

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In this talk I will describe the difficulties encountered in designing materials at the nanoscale and present recent research in which computer simulations are used to guide experiments to create novel materials for devices. I will describe our attempts to decipher design rules for the synthesis of large-area molecular tunnel junctions with giant rectification of electrical current, graphene-based molecular sensors, and piezoelectric amino acid crystals.