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Pongsathon finished his undergraduate study in 2015 and received a Bachelor of Science in Chemistry from Mahidol University, Thailand. His undergraduate project involved chiral resolution of natural-occurring compounds. His two THETA projects at the BCFN involved synthesis of metal oxide for energy applications and computer simulations of nanoantenna systems. His areas of interest are organic synthesis and modification of responsive nanomaterials for use as sensing and indicating materials.

“Synthetic and Computational Studies of Poly(aniline)-Based Conjugated Microporous Polymers”

Conjugated microporous polymers (CMPs) are materials which possess porosity and π -conjugation throughout their structures. These materials are of interest for a range of applications, including carbon capture and utilisation (CCU) technology, adsorption of molecules for storage or segregation, and catalysis. Previous experimental and computational studies have found that properties of linear polyanilines and oligoanilines can be tuned by doping and by simple modification of their structures. Three-dimensional, highly crosslinked polyaniline-based CMPs (PANI-CMPs) are the focus of this study due to their tuneable structures and optoelectronic properties, high nitrogen contents, and ease of synthesis. PANI-CMPs also show excellent CO₂ and I₂ sorption uptake capacities. In this work, several PANI-CMPs have been synthesised from Buchwald-Hartwig coupling reactions of bromoarenes and aminoarenes. Meanwhile, density functional theory (DFT) and time-dependent DFT calculations have been applied to study electronic properties and transitions. Optoelectronic properties, morphology, isotherm adsorption, and porosity of these materials have been investigated. Results from experimental and theoretical investigations are compared, and design rules for further materials development are discussed.