

## CBC SEMINAR ANNOUNCEMENT



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**Quantum chemistry in ligand directed catalysis**

The synthesis of speciality chemicals for various applications — pharmaceuticals, natural products, agrochemicals, polymers — often require methods to activate carbon-hydrogen bonds in one substrate, and subsequently form carbon-carbon, carbon-nitrogen, and carbon-halogen bonds with others. Desirable catalysts offer high product selectivity, wide substrate scope, appreciable yield, and mild operating conditions for these chemical transformations. In collaboration with groups from A\*STAR's Institute of Chemical Engineering & Sciences (ICES) and Singapore Bioimaging Consortium (SBIC), two families of ligands, namely, a meta-terarylphosphine ligand \*Phine, and functionalized thioamides were developed, and analyzed. The \*Phine-directed catalysis of aromatic fluorination, copper-free Sonogashira coupling, and N-arylation, along with the thioamide-directed selective activation of C(sp<sup>3</sup>)-H were investigated using ab initio and density functional methods, results of which will be presented and discussed. Insights from these studies contribute to systematic optimization of ligands that in turn shorten the design cycle of catalysts.

<b>Date:</b>	<b>8th November 2017 (Wednesday)</b>
<b>Time:</b>	<b>2:30pm – 4:00pm</b>
<b>Venue:</b>	<b>SPMS Research &amp; Graduate Studies Office Conference Room</b>
<b>Host:</b>	<b>Asst Professor Loh Zhi Heng</b>