

## CBC SEMINAR ANNOUNCEMENT



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### **Properties of Molecules and Nanoparticles in Complex Environments**

In this talk I will briefly review some ongoing research at our department. I will highlight recent efforts using the integrated quantum mechanics - molecular dynamics approach developed to predict various properties of molecules in solution and complex environments [1-5]. Some results will be discussed on solvatochromatic effects, one- and two-photon absorption for solvent, protein and DNA environments [6], and probe molecule - amyloid fibril complexes. I will also discuss work on nanoparticles, like colloidal quantum dots and upconversion rare-earth nanocrystals, where we combine modelling with experimental measurements for solar cell and bioimaging applications [7-12]

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- [11] M. Molnár, Z. Ning, et al., *Sensors and Actuators B: Chemical*, DOI:10.1016/j.snb.2011.01.055. (2011)
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<b>Date:</b>	<b>31<sup>st</sup> August 2012 (Friday)</b>
<b>Time:</b>	<b>11:00am – 12:30pm</b>
<b>Venue:</b>	<b>NTU SPMS CBC Building Level 2, Conference Room</b>
<b>Host:</b>	<b>Asst Professor Zhao Yanli</b>