Computational Modelling of Plasmonic Biochemical Sensors

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Monday February 25, 11:00, Room MED 2 1124 (CoViz2)

Abstract: Plasmonic biochemical sensors are powerful analytical tools for the detection and measurement of trace pollutants in air and water. There are published reports on ultra-sensitive plasmonic sensors capable of detecting single molecule with marginal amount of analyte. Such striking sensitivity is due to the confinement of localized collective electron oscillation at resonance on the nanostructure surface. The oscillation is very sensitive to local refractive index change due to target-receptor interaction. Yet, it is impossible to build such plasmonic sensors by simply trial-and-error. With computational modelling, it is possible to tackle some of the challenges, i.e. i) design of nanostructures to maximize optical response, ii) enhancement of optical signal for better detection sensitivity, iii) investigation of target-receptor-surface interaction for novel plasmonic supporting materials. As planar nanoscale thin-film, the first two questions can be resolved by calculating the Fresnel's equations analytically provided that the appropriate materials' parameters are known. For discrete nanostructures, i.e. nanoislands and nanospheres, iterative algorithms such as finite difference time domain (FDTD) and discrete dipole approximation (DDA) can be used. The third question requires fundamental exploration of the electronic structure of surface and interacting molecule. This is *N*-body problem involving multiple valence electrons which can be resolved by density functional theory (DFT), a computational quantum mechanical modelling method. The talk will demonstrate some examples involving these techniques for label-free plasmonic sensors, 1) surface plasmon resonance (SPR) with analyte/metal/dielectric nanoscale thin-film structures,

2) a novel gain-assisted surface plasmon-polariton amplifier, 3) a Ni-doped graphene synthetic receptor for label-free detection of amino acid, and 4) a biotinylated functionalization protocol for novel titanium nitride based SPR biosensor.

Bio: Siu Pang Ng graduated from B.Sc. in the Hong Kong Polytechnic University 2003 and obtained his MPhil degree in Optical Metrology for Nondestructive Testing using Shearogrphy in the City University of Hong Kong (CityU HK) 2007. His research in Label-free Surface Plasmon Resonance (SPR) Optical Biosensor started in 2008 with the Department of Physics and Materials Science under supervision of Prof. Chi-man Lawrence Wu. In the PhD period of two consecutive years, he invented the white-light spectral interferometric technique for ultra-sensitive Label-free Surface Plasmon Resonance biosensor with expanded dynamic range of measurement, thus 4 US patents and 2 CN patent were filed and granted based on his invention. Since his PhD graduation 2010, he works as Research Fellow in CityU HK ever since and continues his effort to develop label-free optical biosensor for various applications. The latest advancements include: (1) the replacement of conventional gold material with novel titanium nitride thin-film for SPR biosensors, (2) rapid detection of trace Lead(II) ions in drinking water to 1/1000 World Health Organization guideline threshold using label-free LSPR optochemical sensor, (3) direct detection of tumor-derived extracellular vesicles and differentiation of exosome from micro-vesicles using Self-assembly Gold Nanoislands LSPR biosensor. Thus, he has authored/co-authored 44 papers in high-impact journals in the field of biosensors, optics, and analytical chemistry. He was awarded the outstanding reviewer by Biosensors and Bioelectronics, the leading journal in the field published by Elsevier 2016. He was also invited to serve as reviewer for Chemical Reviews, the top journal in Chemistry, by the American Chemical Society 2018. Most recently, he is also involved in quantum chemistry computation to further elucidate the biosensing mechanism with density functional theory and ab initio molecular dynamics.