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Modelling Driven Discoveries in Molecular Spectroscopy

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A significant number of scientific discoveries in the past was driven by experiment with several exceptions. The coming industry 4.0 era will be digital and computer simulation driven. Physical properties of almost all materials should be predictable, in principle, by solving the quantum-mechanical equations governing their constituent electrons. Such calculations require only a small number of chemical elements in appropriate positions through forces. This presentation will cover a broach spectrum of simulation driven discoveries in recent years at Swinburne University through international collaboration. In particular, the narrative of research collaboration leading to breakthrough of the structure of ferrocene using IR spectroscopy will be presented (University of Melbourne and Australian Synchrotron). The X-ray photoemission spectroscopy (XPS) of biomolecules in collaboration with Elettra-Sincrotrone, Trieste (Italy) will be discussed. I will also present primary results of the recent development on interactions between single molecule and metal surfaces.

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