

Control and characterization of matter on the atomic scale

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The fiction to control matter on the atomic scale is becoming a reality by the unique capabilities provided by the scanning tunnelling microscope (STM) to image, characterize and manipulate single atoms and molecules on surfaces. In this talk I will present some highlights of our on-going theoretical work done in collaboration with the experimental groups of W. Ho, UC Irvine and G. Meyer, IBM Zurich on manipulation and characterization of single atoms and molecules adsorbed on a metal surface by inelastic electron tunnelling in an STM junction. These highlights include (1) single molecule vibrational spectroscopy and microscopy and chemistry; (2) charge state control of single adatoms adsorbed on thin insulating films supported by a metal substrate; (3) characterization of electronic states of vacancies in such films; (4) frontier orbital reorganization in a single metallo-organic complex. Our theoretical approach is based on density functional theory of the electronic structure and a many body extension of Tersoff-Hamann theory to vibrational inelastic tunnelling.