Canadian Association of Physicists
Association canadienne des physiciens et physiciennes

Contribution ID: **2188** Type: **Oral (Non-Student) / Orale (non-étudiant(e))**

# Submolecular scale mapping of the Hubbard U

*Tuesday 12 June 2018 12:00 (15 minutes)*

When orbitals are already occupied by one electron, the addition of a second charge to that position in space entails overcoming the Coulomb repulsion between the charges. This on-site Coulomb repulsion is often characterized by the so-called Hubbard U: the energy difference between the doubly negative and charge neutral state. As charges move from site to site in a material they must overcome this interaction, and when U is large compared to hopping parameters these effects influence transport, breakdown single particle theories, and lead to low temperature phase transitions into distinct electronic states. As these effects are inherently local, and orbital dependent, a real-space tool to measure this on-site Coulomb interaction has the potential to offer new insight into interaction-driven and correlated electron behavior.
Here we provide a new sub-nanometer scale view into this old problem via noncontact atomic force microscopy. Our observations of singly charged 3,4,9,10-peryelene tetracarboxylic dianhydride (PTCDA) molecules on bilayer NaCl on an Ag(111) surface show bias-dependent transient charging behavior. Electrostatic force spectroscopy (EFS) shows distinct jumps at the energies corresponding to Hubbard states previously identified by scanning tunneling spectroscopy (STS) [1] and are indicative of transitions between the 0, 1-, and 2- states. Using pixel-by-pixel EFS in tandem with STS we can locally map this charging energy required to overcome the on-site Coulomb repulsion providing a direct characterization of the Hubbard interaction. Our measurements indicate that the Hubbard U varies spatially depending on the local environment of 2-dimensional clusters of PTCDA molecules and even on submolecular length scales associated with the spatial extent of the half-filled orbital. This new visualization tool has the potential to be applied to a wide range of materials providing opportunities open up new perspectives in this key underpinning of correlated electron behavior.

[1] K. A. Cochrane, A. Schiffrin, T. S. Roussy, M. Capsoni & S. A. Burke, Nat Commun, 8, 8312 (2015)

**Primary author:** Prof. BURKE, Sarah (University of British Columbia)

**Co-authors:** Dr YUAN, Bingkai; Ms ROUSSY, Tanya; Mr TOM, Gary; Dr COCHRANE, Katherine

**Presenter:** Prof. BURKE, Sarah (University of British Columbia)

**Session Classification:** T2-6 Experimental Techniques (DCMMP) | Techniques expérimentales (DPMCM)

**Track Classification:** Condensed Matter and Materials Physics / Physique de la matière condensée et matériaux (DCMMP-DPMCM)