Bar-Ilan University
אוניברסיטת בר-אילן

Faculty of Exact Sciences
Department of Chemistry

הפקולטה למדעים מדויקים
המחלקה לכימיה

S E M I N A R

Monday 11/11/19, 12:00 pm

Building 211, seminar room

SPEAKER:

Prof. Baran Eren

Weizmann Institute of Science

TOPIC:

Surface Science at the Dawn of the 21st Century

Abstract:

Classical Surface Science is carried out under very refined conditions of ultra-high vacuum (UHV) and sometimes at cryogenic temperatures. This approach in Surface Science has provided the core of our present understanding of solid surfaces, thanks to an extensive array of surface-sensitive microscopy and spectroscopy techniques that revealed the atomic, electronic, and chemical structure of crystal surfaces in their pristine state. This type of studies also helped us to understand the structure, thermodynamics, and kinetics of certain model reactions. However, practical catalytic reactions typically take place in the presence of gases (or liquids) at much higher pressures and at room temperature (RT) or above. Today, much of our existing fundamental understanding of surfaces involved in heterogeneous catalysis still relies on studies of model single crystals using surface-sensitive techniques that typically require UHV. Consequently, our knowledge of surfaces under catalytic application conditions remains less extensive than in UHV, because only a few surface sensitive techniques exist that can probe surfaces in the presence of gases at ambient pressure conditions. The term “pressure gap” refers to this discrepancy in our Surface Science doctrine. However, it is more relevant to think of this knowledge gap as made of three different gaps, determined by pressure, temperature, and complexity of the system. The pressure gap is due to the fact that most surface sensitive techniques require high vacuum for operation, because the probe particles, electrons, ions, etc., whether incoming or outgoing, have mean free paths below 1 mm at pressures above a few mTorr. At UHV, however, the high density of adsorbed atoms and molecules, typical of real life conditions, can only be obtained by operating at low temperatures, typically at liquid nitrogen temperature (77 K) and below. However,

under such condition the kinetics of surface processes is too slow for practical experiments to be carried out in practical times of minutes. This is the “temperature gap”, which is very important because kinetics scale exponentially with temperature. In addition to pressure and temperature gaps, “complexity gap” is related to the fact that most practical materials are not single crystals or thin films, but are in the form of powders, nanoparticles, porous media, etc., that put additional barriers to atomic level characterization.

The first part of my talk is about the outcomes of my postdoctoral research at the Lawrence Berkeley National Laboratory. Using pressure scanning tunneling microscopy (HPSTM), we show that the most compact and stable surfaces of Cu undergo massive reconstructions in the presence of CO at room temperature at pressures in the Torr range, and they decompose into two-dimensional nanoclusters, which is a double effect of low cohesive energy of Cu and the high gain in adsorption energy at the newly formed under-coordinated sites. Here we discuss the atomic structure of the nanoclusters as a function of CO pressure, their energetics for formation, and the growth mechanisms, as well as their importance for heterogeneous catalysis. Whilst 19-atom large hexagonal clusters are the building blocks of larger clusters on the Cu(111) surface, linear clusters form on the Cu(100) and Cu(110) surfaces. Surface-sensitive spectroscopy techniques such ambient pressure photoelectron spectroscopy (APXPS) and infrared reflection absorption spectroscopy (IRRAS) are used to corroborate the HPSTM results. The surfaces which are broken up into clusters are more active for water dissociation, a key step in the water gas shift reaction. Such a behavior opens a new paradigm, especially for other soft metals like gold, silver, zinc, etc., and it is clear that we need more of such studies. Similar to CO, CO_2 also breaks up the Cu(100) surface into clusters, however at higher pressures. CH_3OH vapor, on the other hand, does not cause the break-up of Cu into clusters because methoxy already adsorbs strongly on Cu terraces.

In our new group at the Weizmann Institute of Science, we aim to shift to current paradigm in this field as we plan to use our current expertise in Surface Science techniques (those applicable at ambient pressures) for understanding more complex materials such as the reducible and non-reducible oxides, metal/oxide interfaces, bimetallic surfaces, and nanoparticles. In some cases, the existing techniques have to be modified or replaced in order to be applicable to the complex material systems. These techniques and research pathway will be explained in the second part of this talk. The focus of our research is using novel techniques to address important yet unsolved questions in fundamental catalysis and interface science, and developing newer techniques to extend this approach to more complex materials.