

# Special Theory Seminar

Tuesday, February 21, 2017, 5:00 pm

Seaver Science Library, Room 150

*SSC Auditorium next to the library*

## Dr. Agostino Migliore

*Department of Chemistry*

*Duke University*

## Molecular Electronic Structure and Local Chemical Environment: A Toolbox for Nanotechnology

### Abstract:

The electronic structure properties of molecules, and their dependence on nuclear motion and external stimuli, offer an extremely rich toolbox to implement reactions and relaxation processes of nanotechnological relevance. Charge transfer is at the core of enzyme reaction mechanisms; charge relaxation and polarization processes can enable chemical sensing, as well as enhanced solar energy harvesting. Photoinduced bond breaking and formation, or the effect of conformational changes on electronic structure properties, can be exploited to produce molecular switches. First, this talk highlights possible scenarios for the coupling of electron and proton transfer at the core of the catalytic mechanism in mononuclear copper monooxygenases. The second part will focus on charge conduction and energy absorption of molecules in contact with graphene and with inorganic materials, or subject to external perturbations such as electrostatic fields. In most of these contexts, the nuclear motion can act as either a determinant or a perturbation of the required molecular property.

Hosted by Dr. Rosa Difelice

*The scientific community is invited*

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