

# From Interstellar Ices to PAHs

A symposium to honor Lou Allamandola's Contributions to the Molecular Universe  
Annapolis, MD, USA - September 13<sup>th</sup> to September 17<sup>th</sup>, 2015

## INVITED TALK

### Quantum chemical predictions of vibrational and electronic spectra of astrophysical ice analogs: The reaction of C<sup>+</sup> with ice and beyond

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Predictions of vibrational and electronic spectra of astrophysical ices before and after various forms of chemical processing offer independent means to potentially identify characteristic spectroscopic signatures of reactant and product species in ice. In this talk, I will use the C<sup>+</sup> reaction with ice as an exemplar of new protocols intended to demonstrate the accuracy of quantum chemical cluster calculations using Density Functional Theory (DFT) for optimizations and prediction of vibrational spectra and Time-Dependent DFT for prediction of electronic spectra. The talk will also look at the reaction of HCO<sup>+</sup> with water, hydrogen cyanide and isocyanide, and ammonia in ice as path ways to yield formic acid, cyano- and isocyanoformaldehyde, and formamide.