Reunião Anual do INCT-FCx - 2022

De 26 a 29/Outubro de 2022,
Hotel Estância Atibainha, Nazaré Paulista/SP

Theoretical Study of Aerosols of Abundant Atmospheric Biogenics Identified Over the Amazon Rainforest

Authors: Emanuel F. D. Mancio, Douglas S. Gonçalves, Kaline Coutinho

Address: Institute of Physics, University of São Paulo – USP, São Paulo – SP - Brasil

Abstract: In recent decades, the Amazon region has undergone a significant change in the dynamics of land use and occupation. These changes have significantly contributed to the increase in the concentration of aerosol particles and greenhouse gases in the atmosphere. Although there are great advances in research in the environmental area, especially in climate change, the role of biogenic aerosol particles in the atmosphere is a current topic and quite lacking in scientific investigations. Aerosol particles play a fundamental role in the hydrological cycle, as they are known as precursors of cloud condensation nuclei (CCN), which participate together with water vapor to form cloud droplets. More than 60% of the aerosol particles emitted by the Amazon rainforest can act as CCN. Due to the heterogeneity of aerosol particles and the increase in pollutant emissions into the atmosphere in the Amazon region, the need for studies on the effect of aerosols on climatic phenomena, as well as the effect of pollutants on natural biogenic particles, in order to obtain information related to the characteristics of these particles in an aqueous environment in the presence of pollutants, as well as to investigate how pollutants affect the interactions of these particles with water. These studies are important because these polluting particles affect the physicochemical properties of the drops, mainly the surface properties, altering the life cycle of the clouds. In this project, we are carrying out theoretical study of molecular modeling, using quantum calculations and classical computer simulations, of natural biogenic molecules in the presence of pollutants and humidity. Firstly, we calculated electronic properties of isolated molecules. Then, we analyzed its interactions with other molecules in the environment under thermodynamic conditions analogous to cloud drops. Some combinations of biogenic molecules presented spontaneous aggregation and formation of nanoparticles. The dynamics and geometry properties of these nanoparticles were analyzed and discussed depending on its composition and the influence of pollutants and humidity.

Key-words: Aerosols; Organic biogenic molecules; Water Effect.
Support: This study was financed by Brazilian funding agencies FAPESP (grants 2021/09016-3 and 2022/01284-1), CAPES and CNPq