

UNIVERSITY OF MACAU
FACULTY OF SCIENCE AND TECHNOLOGY
DEPARTMENT of
CIVIL AND ENVIRONMENTAL ENGINEERING

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**" Multiphase Chemistry of Organic Aerosols in the
Atmosphere "**

by

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Abstract

Multiphase chemical processes of oxidants and aerosol particles are of central importance in aerosol effects on outdoor and indoor air quality and public health. Kinetic multi-layer models for gas-particle interactions and multiphase chemistry have been developed that explicitly treat mass transport and chemical reaction of semi-volatile species partitioning between gas and condensed phases. These models have been applied to gas uptake and chemical aging of organic aerosols as well as formation and evolution of secondary organic aerosols. Secondary organic aerosols (SOA) are ubiquitous in the atmosphere. SOA can occur in amorphous solid or semi-solid phase states depending on chemical composition, relative humidity (RH), and temperature. The phase state of SOA is important for their effects on climate and air quality, but its global distribution is poorly characterized. Our analysis of SOA phase state builds on the molecular corridor approach, which is a two-dimensional framework of volatility and molar mass of SOA components constrained by boundary lines of low and high molecular O:C ratio. We developed a method to estimate glass transition temperatures based on the molar mass and molecular O:C ratio of SOA components. We predict viscosity from the Tg-scaled Arrhenius plot of fragility as a function of the fragility parameter. Viscosity of toluene SOA was predicted using the elemental composition obtained by high-resolution mass spectrometry (HRMS), resulting in a good agreement with the measured viscosity. Further, we used the global chemistry climate model EMAC with the organic aerosol module ORACLE to predict the phase state of atmospheric SOA. For the planetary boundary layer, global simulations indicate that SOA are mostly liquid in tropical and polar air with high relative humidity, semi-solid in the mid-latitudes, and solid over dry lands. We find that in the middle and upper troposphere SOA should be mostly in a glassy solid phase state. Thus, slow diffusion of water, oxidants, and organic molecules could kinetically limit gas-particle interactions of SOA in the free and upper troposphere, promote ice nucleation and facilitate long-range transport of reactive and toxic organic pollutants embedded in SOA.

Biography

Prof. Manabu Shiraiwa is Assistant Professor of Chemistry at the University of California, Irvine. He has worked as group leader at the Max Planck Institute for Chemistry and as JSPS postdoc fellow at the California Institute of Technology. He received BS and MS at the University of Tokyo and PhD from the Max Planck Institute for Chemistry. He has published > 70 papers, with a total citation of >3500 and an h-index of 30 in Web of Science. He is the awardee of the NSF CAREER Award of National Science Foundation (NSF), the Sheldon K. Friedlander Award of American Association for Aerosol Research (AAAR), the Paul-Crutzen Prize of German Chemical Society, and the Otto-Hahn Medal of Max Planck Society.

ALL ARE WELCOME!