Contribution ID: **7** Type: **not specified**

Broadband and Molecular Dynamics Analysis of Propylene Carbonate and its Binary Mixtures with Alcohols

Wednesday, 13 March 2024 14:15 (5 minutes)

This study explores the dielectric properties and relaxation behaviors of propylene carbonate (PC) and its binary blends with methanol and ethanol. Utilizing a coaxial-circular cutoff waveguide junction, broadband dielectric spectra (0.1 GHz to 18 GHz) were characterized, employing a two-group Debye model to extract relaxation parameters. Analysis of excess thermodynamic parameters, Kirkwood orientational correlation factors, and Bruggeman factors for PC-alcohol mixtures was conducted. The data offer insights into microscopic processes, such as the disassociation of alcohol hydrogen-bond networks, formation of new PC-alcohol networks, parallel alignment of dipoles, and enhanced dielectric effects with increasing PC concentration. Molecular dynamics simulations using the TraPPE-UA forcefield exhibited good agreement with experimental results, highlighting the gradual formation of PC-cage and alcohol-cluster microstructures in PC-rich mixtures. These findings hold potential practical applications in high-energy batteries and the pharmaceutical industry.

Primary author: TSAI, Shang-Da

Co-authors: YAO, Hsin-Yu (Department of Physics, National Chung Cheng University); CHANG, Tsun-Hsu (Department of Physics, National Tsing Hua University)

Presenter: TSAI, Shang-Da

Session Classification: Poster

Track Classification: Poster section