Refractive index spectroscopy of ionic liquids: experiments and simulations

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In this contribution we present a summary of different experimental and computational techniques to study the refractive index of ionic liquids (ILs) as a wavelength-dependent magnitude [1,2]. From the experimental perspective, we present a novel technique, Refractive Index Spectroscopy by Broadband Interferometry (RISBI), as a method for determining the refractive index of ILs as a continuum function of the wavelength in a broad spectral range. We measured the refractive index dispersion for the $[C_k mim][BF_4]$ family of ILs with k=2-10, Fig. 1. The results were modeled it in terms of a three-resonance Sellmeier equation and compared with the predictions from density functional theory (DFT) calculations, which provides valuable insights into the relation of the refractive index and electronic polarizability dispersion with the structure of ILs.

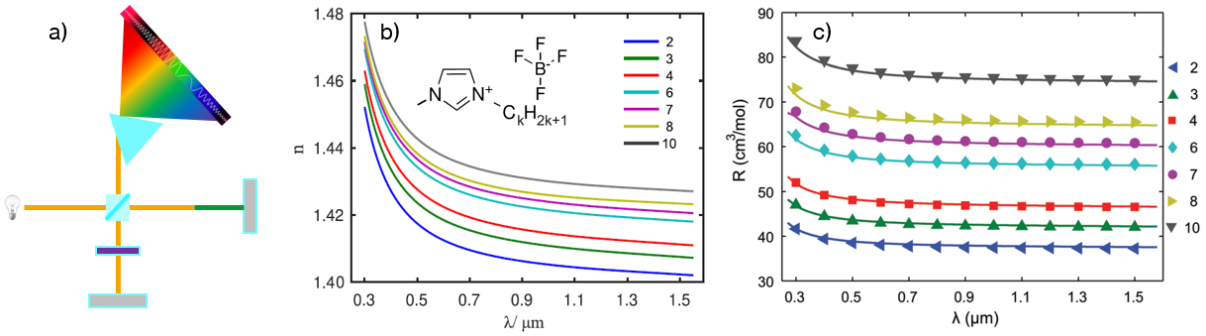

Fig.1 a) RISBI experimental scheme b) refractive index dispersion measurements of the $[C_k mim][BF_4]$ family with k=2-10 c) comparison with DFT simulated molar refractivity dispersion.

On the other hand, a general ab initio method for predicting the refractive index of ILs is presented and its performance compared with experimental results. The simulations draw a map of the distribution of refractive index in the world of ILs and point towards new strategies, namely charge transfer tuning, to tailor the refractive index in ILs beyond the standard ranges of values.

Bibliography

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