THE ELECTRONIC STRUCTURE OF GAS PHASE IONIC LIQUIDS CONTAINING TFSI ANIONS

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Valence electronic structure of three ionic liquids (ILs) with bis(trifluoromethylsulfonyl)imide (TFSI) anion (also called as bistriflimide (Tf_2N)) is under investigation in the present work: 1-Butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)imide ([$PYR_{1,4}$][TFSI]), diethylmethyl (2-methoxyethyl)ammonium bis(trifluoromethylsulfonyl)imide ([DEME][TFSI]) and (1-Ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([EMIM][TFSI]).

The synchrotron radiation excited photoelectron spectroscopy measurements of gas-phase ILs were carried out at the FinEstBeAMS beamline of the MAX-IV 1.5 GeV synchrotron storage ring (Lund, Sweden) [1]. The beamline covers the photon energy range from 4.5 eV to about 1300 eV. The spectra were measured with excitation energy 40 eV. Binding energies were calibrated to Ar $3p_{3/2}$ (15.76 eV) photoelectron lines [2]. For interpretation the density functional theory calculations were performed. The comparison of experimental and calculated results shows large contribution of the TFSI anion to the valence band.

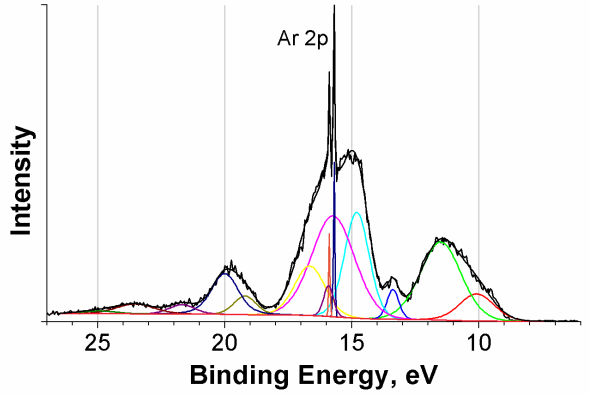

Fig.1. Valence band spectrum of [EMIM][TFSI] fitted with density functional theory calculated peak positions. Argon was dosed in for energy calibration.

References

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