Local and Symmetry-Resolved Electronic Structure of Liquid Dimethyl Sulfoxide from Resonant Inelastic Soft X-ray Scattering

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Dimethyl sulfoxide (DMSO, C_2H_6OS) is a highly polar solvent with comparatively low toxicity. It is used in many fields to dissolve a wide range of both polar and non-polar organic and inorganic compounds. The unique properties of DMSO are strongly defined by the sulfinyl functional group, in which the nature of the bond between sulfur and oxygen plays a central role. A detailed understanding of DMSOs electronic structure is crucial, and advanced soft x-ray spectroscopy techniques now allow to study such molecular systems also in the liquid state. In our contribution, we derive the local and symmetry-resolved electronic structure of liquid DMSO, using resonant inelastic soft X-ray scattering (RIXS) maps at the S $L_{2,3}$, C K, and O K edges. Such maps give the most complete experimental description of the electronic structure of this important solvent, especially when combining them with calculations based on density functional theory that enable a detailed locally- and symmetry-resolved analysis of the molecular orbitals. In the RIXS maps, we find the signature of molecular-field splitting of the S 2p core levels, vibronic coupling, and ultrafast nuclear dynamics on the time scale of the RIXS process.

[1]L. Weinhardt, D. Hauschild, R. Steininger, C. Wansorra, W. Yang, and C. Heske, *"Local and Symmetry-Resolved Electronic Structure of Liquid Dimethyl Sulfoxide from Resonant Inelastic Soft X-ray Scattering"*, J. Phys. Chem. Lett. (12) 10576 (2024).

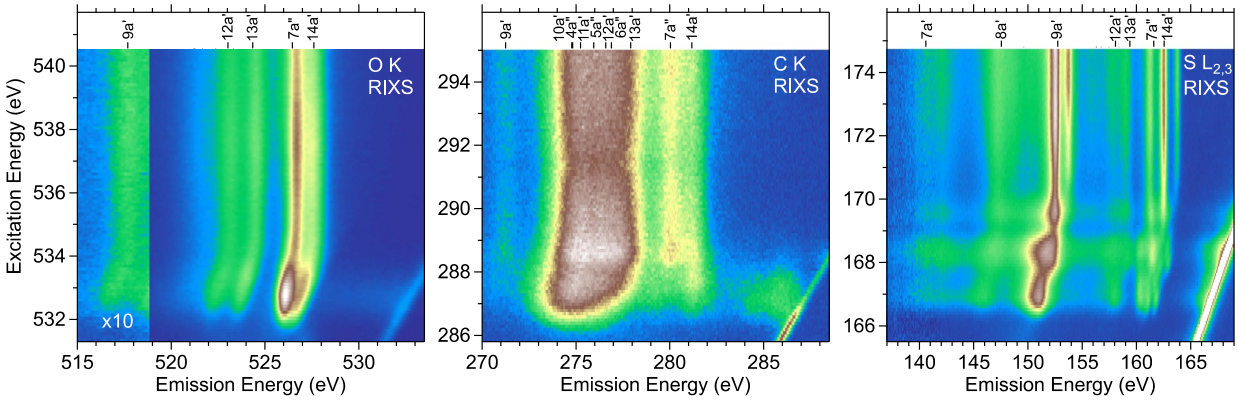

Figure 1. O K (left), C K (center), and S $L_{2,3}$ (right) RIXS maps of liquid DMSO. Above the maps, emission lines are labeled and marked according to their calculated non-resonant emission energies. From Ref.[1]