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New approaches towards efficient optical materials: Dyes and organometallic complexes dispersed in sol-gel mesoporous hosts.

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Sol-gel silicate glasses and ordered mesoporous materials containing luminescent species such organic dyes and lanthanide and transition metal complexes have lately been at the focus of much attention for optical device and bioanalytical applications. In all these applications, and particularly for the latter, it is very important to assure high luminescence efficiency while avoiding contamination of the surrounding environments by leakage of the active species from the mesopores. In this sense, the sol-gel silicate hosts with high surface areas and easy functionalization offer vast possibilities to disperse the guest molecules so as to avoid, or at least decrease, the formation of non-emissive molecular aggregates (as it is common for dyes), and to protect them from exposure to well known luminescence quenching agents such as OH- (for most lanthanide complexes) and singlet oxygen (e.g. for iridium complexes). Lately, our research group at the University of São Paulo has dedicated efforts to the development of several host-guest materials, as above cited, and studied them from the structural and photophysical points of view. Examples include ordered mesoporous silica (MCM-41), organo-modified silica xerogels, and sodium-aluminophosphate glasses incorporated with Rhodamine 6G dye, Ir(III) and Eu(III) complexes. For each case, new approaches are designed to achieve host-guest interactions leading to high dispersion of the guest molecules and avoidance of leakage. As a general rule, all the materials obtained presented remarkable improvements of photophysical properties such as excited state lifetimes and quantum yields, when compared to the values obtained for the molecular species in solutions. Besides preserving the environment to each they are exposed, the incorporation of the emissive molecules in the solids also suggests an increase in the operational lifetimes of devices (not tested). In order to probe the host structure (beyond analysis through FT-IR, SAXs and N2-sorption), the distribution and concentration of luminescent species, and host-guest interactions, high resolution solid state NMR of the nuclei 1H, 29Si, 23Na, 27Al and 19F was largely employed. The optical-spectroscopic data was obtained from emission, absorption, excitation, lifetime and quantum yield experiments and, whenever possible, structural-functional correlations were sought.