# Highly luminescent ionic liquids and ionogels with Pt(II) complexes: Photophysics and insights on molecular aggregation by DFT analysis.

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## Abstract

In this work, we report the preparation and structural/photophysical characterization of luminescent silica ionogels based on a water soluble neutral Pt(II) complex with possible application in luminescent devices. Complementary, the extent of molecular aggregation, which influences emission properties, was approached by theoretical analysis through DFT.

## Introduction

Luminescent materials based on Pt(II) complexes have been studied with great interest for applications in luminescent devices such as OLEDs and LEECs. The reason lies in the fact that these complexes are triplet emitters with efficiency close to 100%. In this work we report the preparation and characterization of luminescent silica ionogels based on a water soluble neutral Pt(II) complex (see structures below).

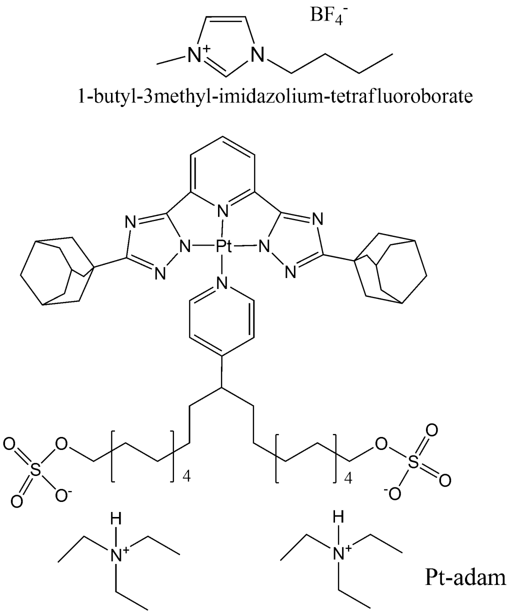

**Figure 1.** Chemical structures of the ionic liquid and the Pt(II) complex.

## Results and Discussions

The presence of the ionic liquid in the sol-gel reaction has a major impact on the optical properties of the complex. First, it acts as a strong catalytic agent, such that the silica network has a high degree of polymerization in short aging times (in a couple of minutes). Second, it induces complex aggregation, a prominent strategy to obtain highly luminescent species. The studies were conducted by employing different spectroscopic techniques combined with density functional theory (DFT), in which molecular coupling and chemical environments were explicitly accounted. This challenging quantum chemical studies were conducted using recently developed DFT approaches, namely: Dispersive forces were introduced by the semi-empirical dispersion correction DFT-D3 developed by Armbruster et al.[1] Excited states were obtained on the framework of time-dependent DFT using the range separated hybrid functional ωPBE, optimized for each particular system by enforcing that the first ionization energies and the Kohn-Sham frontier orbital eigenvalues agree as closely as possible.[2]

## Conclusions

With the applied methodology we could describe long-range intermolecular interactions and charge transfer excitations, crucial effects on the photophysics of Pt(II) complexes and aggregates. It is demonstrated that the aqueous and ionic liquid solutions, as well as the xerogels and ionogels, contain simultaneously monomers and aggregates, and that energy transfer from the monomer to the aggregates has a higher rate than the monomer emission, favoring the luminescence efficiency, in agreement with recent findings.[3]

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