Using organic magnetoresistance effect features to understand the spin-orbit coupling in rareearth quinolinate complexes effect based devices

<u>Rafael dos Santos Carvalho</u>¹, Deyse Costa², Harold Camargo Ávila¹, Tiago Becerra Paolini³, Hermi Felinto Brito³, Rodrigo B Capaz⁴, Marco Cremona¹

¹Pontifícia Universidade Católica do Rio de Janeiro, ²Universidade Federal de Viçosa, ³Instituto de Química, USP, ⁴Universidade Federal do Rio de Janeiro

e-mail: rafael.santos@fis.puc-rio.br

Organic Electronics plays an important role in innovation and technology market. Most of it was only possible due to the understanding of fundamental physical and chemical properties of the materials used to perform efficiency devices. Recently, a spin-dependent mechanism of the charge transport in organic semiconductors (OS) was observed via the so-called OMAR (Organic Magnetoresistance Effect) [1]. So far, it is known that hyperfine interactions (HI) (especially hydrogen) play an important role in this phenomenon and also that spin-orbit coupling (SOC) is negligible for light-atom based compounds [2]. In this study we used a family of rare-earth guinolinate based complexes, as active layers, that presents a new feature in the OMAR curves to evidence the influence of the spin-orbit coupling mechanism on charge transport. Those tetrakis 8-hydroxyquinolinate complexes have been chosen because their optical, electrical and magnetic properties similar to the Alq₃ molecule widely reported in literature [3]. Electronic structure calculations based on density functional theory (DFT) help to establish the connection between the results and the presence of heavy central ions in the different complexes. Here we have observed a non-Lorentzian type curve with two physical parameters (B and B_1) correlated with HI and SOC, respectively, which the B_1 scales with the atomic number of the RE^{3+} ion. This result reviews an important aspect of the charge transport mechanism in organic semiconductors. The combination of experimental and theoretical methods provides a strong and clear evidence of spin-orbit effects in the charge transport mechanism for the used rare-earth guinolinate based complexes.

[1] Marco Gobbia and Emanuele Orgiu, Journal of Material Chemistry C, (2017).

[2] R. Giro at al., Physical Review B 87, 125204 (2013).

[3] M.A. Guedes at al., Journal of Luminescence 131, 99, (2011).