

Modelling persistent luminescence: theory vs. experiment

J. Hölsä^{1,2}, H.F. Brito³, T. Laamanen^{1,4}, M. Lastusaari^{1,2}, M. Malkamäki^{1,4} and
L.C.V. Rodrigues^{1,3}

¹*University of Turku, Department of Chemistry, FI-20014 Turku, Finland*

²*Turku University Centre for Materials and Surfaces (MatSurf), Turku, Finland*

³*Universidade de São Paulo, Instituto de Química, São Paulo-SP, Brazil*

⁴*Graduate School of Materials Research (GSMR), Turku, Finland*

Already the very idea of generating strong luminescence continuously for up to 24 hours after ceasing the excitation upon a material gives strong incentive to the human curiosity – in addition to its important commercial applications. All this despite the fact that persistent luminescence has been known since the beginning of the 17th century: the persistent emission from the famous Bologna Stone has been left unexplained up to date. So far, both the development of new persistent luminescence materials as well as tailoring of the existing ones to reach enhanced properties has been carried out on the trial and error basis. The undisputable success of such an experimental approach leaves, however, no doubt that the full potential of these materials has not yet been exploited. The use of theoretical methods in the development of persistent luminescence has been indeed very feeble so far. The reasons for this unfortunate state of affairs can probably be found in the multidisciplinary nature of the phenomenon: solid state chemistry as well as physics is not quite enough to design new materials but materials engineering together with sophisticated spectroscopy are required, too. At present it is known that efficient persistent luminescence cannot be achieved without efficient photoluminescence. Thus such strong emitters as Eu^{2+} , Ce^{3+} or Tb^{3+} and Mn^{2+} are found as the emitting centre. In addition to the emitting centre, the host lattice of the luminescence material is as important – or, as in the case of persistent luminescence, even more important – as the emitter. The hosts found among the most efficient persistent luminescence materials include different complex silicates (*e.g.* $\text{Sr}_2\text{MgSi}_2\text{O}_7$), aluminates (*e.g.* SrAl_2O_4 and $\text{Sr}_4\text{Al}_{14}\text{O}_{25}$) or even simple oxides as Lu_2O_3 . The host lattice should be stable and rigid enough to allow efficient luminescence but, at the same time, easy to be modified *e.g.* by co-doping with ions with a charge incompatible with those of the host ions, *e.g.* trivalent rare earths (R^{3+}).

Eventually, the interplay between the luminescence centre and the host lattice should not be overlooked either. The energy level scheme of the luminescence centre should be suitable to allow the transfer of the charge carriers to the host and to the traps. The interplay should also enable the emitting centre to change its charge, or at least to form complex ion – charge carrier species.

In this contribution, the up-to-date theoretical methods to model and enhance the properties of the persistent luminescence materials are reviewed.

Keywords: Persistent luminescence, rare earths, Density Functional Theory

Work supported by the European Union, CNPq, FAPESP and the Academy of Finland.

jholsa@utu.fi; University of Turku, Department of Chemistry, FI-20014 Turku, Finland.