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# The electronic structure of Tl, Pb, and Bi based scintillators and how that relates to scintillator performance

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The Sr co-doped LaBr3:Ce3+ scintillator is an almost ideal scintillator regarding energy resolution and speed. However, its relatively low density limits application in various fields. To develop scintillators with density higher than 8 g/cm3 one has to abandon the research field of the halides, and instead explore oxides containing high Z-cations like Hf, Ta, W, Tl, Pb, or Bi. The question then arises whether Ce3+, Tl+, Pb2+, or Bi3+ will scintillate in those type of compounds? To answer this, one needs to know the electronic structure. Where are the activator excited and ground state levels with respect to the host valence band and conduction band? The chemical shift model, that was developed in 2012 [1], enables to determine the electron binding energy in lanthanide impurity levels with respect to the vacuum. Recently we applied the model to obtain information on the vacuum referred binding energies (VRBE) of Tl+, Pb2+, and Bi3+ in luminescent phosphors [2]. An overview of the results will be presented, and we will explain why Ce3+ does not scintillate in Pb-, Bi-, Ta-, W-based compounds, and why it does scintillate in Tl2LaCl5:Ce [3] and BaHfO3:Ce. We will also address the possibility for Bi to luminesce in Pb- or Tl-based compounds or Pb2+ in Tl- or Bi-based compounds.

[1] P. Dorenbos, Phys. Rev. B85 (2012) 165107
[2] R.H.P. Awater, P. Dorenbos, J. of Lumin. 184 (2017) 221.
[3] H.J. Kim, Gil Rooh, Sunghwan Kim, J. of Lumin. 186 (2017) 219.

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