Contribution ID: **191** Type: **Oral presentation**

A Theoretical First-principles Investigation of the Properties of Self-Trapped Excitons and Defects in Halide Scintillators

Tuesday 19 September 2017 15:15 (15 minutes)

The performance of new and improved materials for gamma ray scintillator detectors is dependent on multiple factors such as quantum efficiency, energy transport etc. In halide scintillator materials the energy transport is often impacted by both intrinsic hole and electron traps such as Vk centers and their associated self-trapped excitons (STE) as well as traps associated with defects and impurities. Recently there has been enormous progress in the development of quantum mechanical methods that allow us to investigate quantitatively these mechanisms. Here we present first principles calculations at the hybrid density functional theory level for the structure, mobility and optical properties of self-trapped excitons in three important families of scintillator materials, the alkali metal, lanthanum and barium halides. Alkali metal and lanthanum halides have been extensively characterized from an experimental point of view and serve in our studies as reference systems to assess the accuracy and reliability of our theoretical procedure. We show that hydrid density functional theory can accurately predict the different types of self-trapped excitons (on and off-center) found in these materials in agreement with EPR experiments. We present results of accelerated molecular dynamics to determine the migration pathways of excitons followed by nudged elastic band method calculations based on the migration pathways to determine the energy barriers to migration. This methodology was then used to perform studies of these defects in new scintillator materials including the barium mixed halides that we will compare to new experimental results.

This work is supported by the Department of Energy, National Nuclear Security Administration, Office of Defense Nuclear Nonproliferation Research and Development and carried out at Lawrence Berkeley National Laboratory under contract #AC02-05CH11231. This work does not constitute an express or implied endorsement on the part of the government

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Session Classification: Scintillation Mechanisms

Track Classification: S07_Mechanisms 1 (Orals)