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A density functional theory and magnetic resonance studies of radiation damage in plastic scintillators

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**Abstract content (Max 300 words)
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Plastic scintillators placed in particle detectors like the ATLAS detector in the Large Hadron Collider undergo structural damage when they interact with energetic particles they detect. This interaction causes damage to the optically active molecules responsible for the scintillation mechanism, affecting the efficacy of the plastic scintillator. In this study we attempt to understand radiation damage in plastic scintillators using a computational density functional theory (DFT) approach to interpret the results of Electron Paramagnetic Resonance (EPR) techniques. This should give insight into the structural damage within the plastic scintillator. Optical absorption and emission properties of the optically active molecules at the DFT, GW and BSE levels will be discussed and the electron hole interaction strength of excited states will be estimated. Calculated hyperfine parameters will be used in an attempt to interpret the width of the measured EPR signal.

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Yes

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 (Hons, MSc,
 PhD, N/A)?**

MSc

**Main supervisor (name and email)
and his / her institution**

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Yes

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