Study of point defects associated with phosphorus by theoretical and experimental spectroscopic coupling

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Abstract

We characterize phosphorus-related defects in glasses by experimental and theoretical approaches. The original approach is to incorporate hypotheses obtained from experimental measurements on irradiated phosphate glasses into the modeling of the structure of P-point defects in order to be able to reproduce by calculations the spectroscopic signatures of unknown defects. The strength of the proposed theoretical-experimental approach is to be able to provide responses on dopant-related defect precursors by characterizing them via ab inito calculation of their optical absorption spectroscopic and EPR signatures while simulating their formation mechanism (precursor nature).

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