Photodegradation in polysilanes

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Abstract

Ultraviolet (UV) or near-ultraviolet (NUV) emission in polysilanes stimulates an interest in utilizing these materials for organic light emitting diodes (OLED) for full colour display through excitation of phosphors/dyes. However, the lifetime of these devices is quite poor in comparison to the existing inorganic UV light emitting diodes (LEDs). Our focus is to understand the photodegradation of the emissive polysilane which is inherent to the material. First, a theoretical understanding is developed by performing the ab initio calculations for a set of model polysilanes. The excited state calculations on model polysilanes explain the relative stability among various polysilanes due to electronic structure and show a dependence of the side groups on the degradation. Besides the electronic structure of polysilanes, the degradation is also a strong function of the environment and morphology. In this regard, we investigated the photdegradation behaviour of a diphenyl-methylphenyl-polysilane copolymer. The degradation of polysilane films in vacuum and air indicate a key role of environment in the degradation process. A model is proposed to explain the kinetics of polysilane degradation in solution and film form. The degradation in film is bi-exponential representing two different sites that lead to two decay rates in photoluminescence (PL). However, in solution we find a single exponential decay in the PL intensity upon UV exposure. Further, the effect of light intensity, excitation wavelength on photodegradation in film is examined.