Identifying the substituent for dehydrogenation of dibenzyl toluene

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Abstract
Liquid organic hydrogen carriers (LOHCs) have attracted attention owing to their advantages in the storage and transport of hydrogen at ambient conditions. Dibenzyl toluene (DBT) has been considered as one of the most promising LOHC candidates. However, the hydrogen release from the hydrogen-rich form of DBT occurs at high temperatures. In this study, the effect of various substituents on the dehydrogenation of DBT was elucidated using density functional theory (DFT) methods. In specific, the charge distribution of DBT was investigated to understand the effect of the modified DBT. This study will be useful for facilitating the use of DBT as a LOHC.
Keywords — Dibenzyl toluene, density functional theory, liquid organic hydrogen carriers