

Title

Betanidin isomerisation and decarboxylation, thermodynamic and charge transfer dye properties towards DSSCs application

Abstract

Along with attractiveness of natural dyes for solar technologies, the instability is a well-known drawback of the dyes which impedes their usage for DSSCs application. Betanidins belong to red-purple pigments betacyanins which experimentally demonstrated good adsorption in a visible range. In this study, the structural, thermodynamic and optoelectronic properties of betanidins have been determined from DFT and TD-DFT computations. On the basis of the thermodynamic approach, isomerisation reaction between two structural conformers of betanidin, bent and planar, and also decarboxylation reaction have been analysed. The planar isomer appeared to be predominant in equilibrium vapour despite its less energetic stability; both betanidin molecules exhibit an inclination to decay into decarboxylated betanidin and CO₂. As for worthy optoelectronic properties and applicability in DSSCs, the dye molecules considered satisfy most requirements to sensitise the semiconductor TiO₂ and be regenerated by electrolytes.