**Link:** <https://solar-power-tech.com/e-posters/dsc_eposter_02/>

**Abstract**

Along with the attractiveness of the betacyanin natural dye for solar technologies, the existence of the 50:50 mixture to both zwitterionic and non-ionic betanidin is of interest to the significant investigation. The instability of structures, which lead to insufficient preliminary information for the requirement to satisfy to be applied to the DSSCs, were sorted out. The conformers are analysed through thermodynamic functions, reactivity indices, and energy level diagrams to understand Gibbs free energies, ground and excited-state oxidation potentials of the dye. Based on the thermodynamic approach, the feasibility of the dimerisation reaction was analysed for both betanidin and decarboxylated betanidin. The non-ionic structures are found to influence the stability of the molecule than the zwitterionic one. The presence of the non-ionic group led to the predominant equilibrium vapour over the zwitterionic case through isomerisation reaction. The noticeably increase to the excited state lifetime to the DSSCs to dimer a range of 59 ns to 184 ns than monomer a range of 2.9 ns to 4.1 ns when CAM-B3LYP functional was used. The lower chemical hardness (h) association to the dimer dye increases the spontaneity ‒ΔG(*T*) of the reaction. As per energy level, effective electron injection is achieved when excited-state potential lies below the LUMO of the dye that becomes successful to the dimer in all dyes under study. The great improvement to the dimer structure is realised than that of monomer, and we expect that most of the challenges to betacyanins will be sorted out.