

DFT Benchmarking of Eumelanin-Inspired Small Molecules

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The high conjugation within the natural pigment molecule, eumelanin, is what gives it the ability to absorb UV radiation. Thus, molecules that apply eumelanin as a core component allow for the preparation of an optimal semiconductor. In order to determine the optimal functional and basis-set pairings that can be used to later calculate HOMO, LUMO, and optical band gap information about these molecules, a benchmarking process took place by combining a variety of different GGA and GH functionals and basis-sets. The results of this study are presented here.