Computational insights into the structure-property relationships in a comprehensive dataset of C_{20}-C_{60} fullerenes

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Fullerenes, as representatives of carbon nano-materials, hold immense untapped potential across numerous applications such as solar energy harvesting, biomedical applications, and catalysis. A given fullerene molecule can exist in various isomeric forms, each showcasing unique structures and properties. Computational studies on fullerenes have rapidly gained attention for their role in elucidating these fundamental characteristics. However, there remains a notable gap in systematically screening and benchmarking density functional theory (DFT) functionals to fully understand and utilize these materials. In this study, we have constructed the most comprehensive computational datasets for C20-C60 fullerenes, encompassing a total of 5770 structures. Through benchmark studies, we provided accurate fundamental properties at the DFT-level and assessed the correlation among stability, electronic properties, and solubility. To further explore the nature and origin of these properties, we introduced various topological indices and geometrical measures, expanding beyond the commonly used isolated pentagon rule. For the first time, our study provides profound insights into the structure-property relationships among diverse fullerene isomers of varying cage sizes, ranging from C20 to C60 and beyond. This work lays a fundamental basis for future advancements in the functionalization and practical applications of fullerenes in the fields of energy conversion and nanomaterials sciences.