

# KEY FACTORS GOVERNING THE RELATIVE STABILITY OF CHARGED, ENDOHEDRAL AND EXOHEDRAL FULLERENES

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Fullerene anions and cations, as well as endohedral and exohedral fullerenes, have unique structural, electronic, and chemical properties that make them substantially different from pristine neutral fullerenes. The theoretical prediction of the most stable structures is a very challenging task due to the large number of isomeric forms accessible (e.g., more than 20 billion isomers for  $C_{60}X_8$ ). In this talk, we present a simple model, exclusively based on topological arguments, that allows one to predict the relative stability of fullerene species without the need for expensive electronic structure calculations or geometry optimizations. The model was first proposed to describe the stability of charged fullerenes[1] and further extended to predict the relative stability of regioisomers in exohedral fullerenes[2]. Very recently we have shown that the model can also predict the reactivity of fullerenes and correctly describe the regioselectivity of Diels-Alder cycloadditions to empty fullerenes[3].

This model allows also identifying the key structural motifs that explain the fullerene stability of charged fullerenes[4], giant neutral fullerenes[5] and the reactivity of empty fullerenes[3]. We show that the subtle interplay between  $\pi$  delocalization, cage strain, and steric hindrance is responsible for the stability of these compounds[6]. The most stable structures predicted by the model are in good agreement with those found in synthetic experiments performed in high-energy conditions. The model has been recently implemented in the code **FullFun** for a widespread use by the fullerene community [7,8].

We have also proposed different reactivity descriptors to predict the most reactive bonds in fullerenes and start to explore the use of these models to predict the reactivity of PAHs.

## References

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