Investigation of several methodologies for simulating the fullerene growth in the presence of hydrogen

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Fulleranes, hydrogenated small fullerenes (C_n, n=20, 24, 26, ..., 52), are a family of polycyclic aromatic hydrocarbons (PAHs), which may play an important role in the carbon cycle in space. Observations revealed that fullerenes are abundant in hydrogen-containing stars[1–4], which suggests hydrogenation may catalyse the fullerene growth by stabilising fused-pentagons. However, theoretical investigation of all the possible structures needs huge computational costs due to a large number of fullerene isomers.

In this study[5], we investigated several parameters and rules that could be used to solve the above computational problem. We found that "single factor" geometric and electronic structure rules for sequential hydrogenation are not able to predict the most stable structures. Rapid empirical and semi-empirical methods are benchmarked against DFT-LDA calculations. We found that the GFN2-xTB extended tight binding method [6,7] consistently reproduces the DFT structures and energetics reducing the calculation speed by a factor of up to one thousand compared to DFT-LDA calculations. Finally, we performed "brute force" testing for all the possible hydrogenated structures up to +4H of two isomers of C_{28} and C_{40}. By this approach we found several prediction rules for the structures of stable hydrogenated small fullerenes.

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