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Original scientific paper submission for the Journal of the Serbian Chemical Society

Dear Editor,

on behalf of myself and my co-author Stefan Grimme, I am pleased to submit our manuscript "Efficient structural and energetic screening of fullerene encapsulation in a large supramolecular double decker macrocycle". In the manuscript we present the theoretical investigation of an organometallic double decker macrocycle for encapsulating fullerene C₇₀, using the recently developed GFN2-xTB tight binding electronic structure method. The computational result is compared to an experimentally measured association free energy. Further we demonstrate the robust GFN2-xTB method in screening 724 higher fullerene isomers for fullerenes up to C₁₀₀ and determine the best binding guest to the supramolecular macrocycle. Our protocol is easily applicable, has low computational cost and is, due to the consistent parametrization of the GFNn-xTB methods, possible for the whole periodic table (up to Z = 86). The authors also state, that none of the material has been published or is under consideration elsewhere, including the Internet.

We suggest the following reviewers:

Prof. Dr. F.M. (Matthias) Bickelhaupt; Vrije Universiteit, Amsterdam

Prof. Dr. Kendall N. Houk; University of California, Los Angeles

Sincerely yours,

Fabian Bohle, M.Sc.