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# Computational Design of Novel Building Blocks for Nanotechnology Based on Core-Modified Metalloporphyrins

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The sizes, shapes, electronic properties, and binding abilities of metalloporphyrins can be broadly tuned by replacing one or more pyrrole nitrogens with other elements, for example, C, Si, chalcogens (O-Te), or P. This type of the porphyrin core-modification is a highly promising approach for tuning the properties as well as reactivity of porphyrin species. Also, metalloporphyrins are able to form numerous covalently and non-covalently linked arrays/stacks with each other as well as complexes with fullerenes and semiconductor nanoparticles (NPs). These building nanotechnology blocks have been extensively explored due to their tremendous potential in applications such as photovoltaic dyes, near-infrared dyes, nonlinear optical materials, nanoelectronics devices, medicine, etc. Stimulated by these facts, along with our recent reports on metalloporphyrins with all the four N's replaced with P, $MP(P)_4$, M = Sc-Zn [1-4], we formulated the following extremely interesting questions to be addressed: (i) Could core-modified porphyrins form stacks without any linkers/substituents? (ii) How strong will core-modified porphyrins interact with fullerenes? (iii) Are core-modified porphyrins able to make complexes with NPs? We present the recent results of the computational design of several novel building nanoblocks based on core-modified metalloporphyrins: (i) stacks; (ii) complexes with fullerenes; and (iii) complexes with small semiconductor NPs and small metal clusters.

**Key-words**: porphyrins, core-modification, nanotechnology, complexes.
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