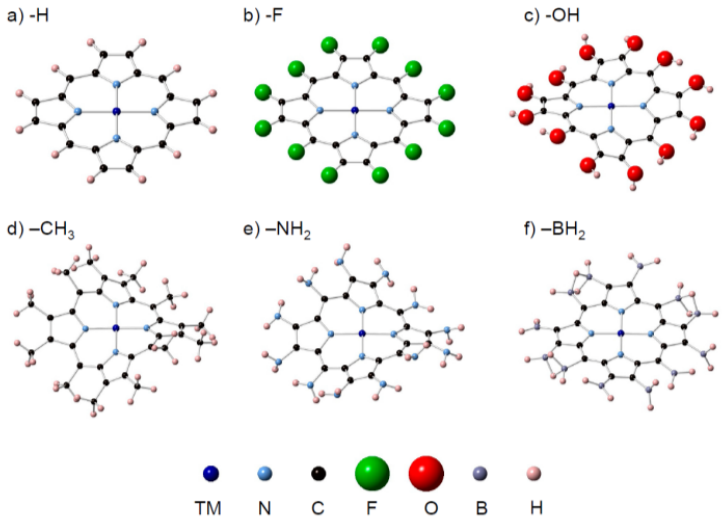
Computational study of phtalocyanines **and porphyrins as catalysts for fuel cells and electrolyzers.**

Challenge: A widespread use of fuel cells and electrolyzersrequires the solution of two fundamental issues: the inefficient electrocatalysis at the oxygen electrode and the elevated price of the electrocatalysts. On the one hand, the oxygen reduction reaction (ORR) at the cathode is known to be the main source of losses in fuel cells. Due to the limited supply and the high cost of platinum, the most common ORR electrocatalyst, the efforts in the field of electrocatalysis are currently focused on the development of two kinds of materials: (1) alloys of non-precious and/or abundant metals with platinum, and (2) inexpensive, stable and active cathode materials, such as porphyrins. In the case of the oxygen evolution reaction (OER) the situation is comparable, given that RuO_2 and IrO_2, the best oxygen-evolving electrocatalysts, are rather expensive and also have large overpotentials.

Idea: Several studies have suggested that porphyrins and phtalocyanines (both organic molecules with a transition metal ion acting as active center for OER/ORR) could potentially show similar activity to the one of the state-of-the-art catalysts. Porphyrins and phtalocyanines have two advantages with respect to traditional catalysts, namely: (1) They are made from cheap and abundant elements, and (2) it is possible to tune their catalytic activity by functionalizing them with side and axial groups.

Your task: You will carry out computational simulations of thin films of porphyrins and phtalocyanines to study their viability as OER/ORR catalysts.



Schematics of the ground-state configurations of the porphyrin rings with various side ligands.

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