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MOLECULAR CATALYSTS THAT OXIDIZE WATER TO DIOXYGEN

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ABSTRACT 1:

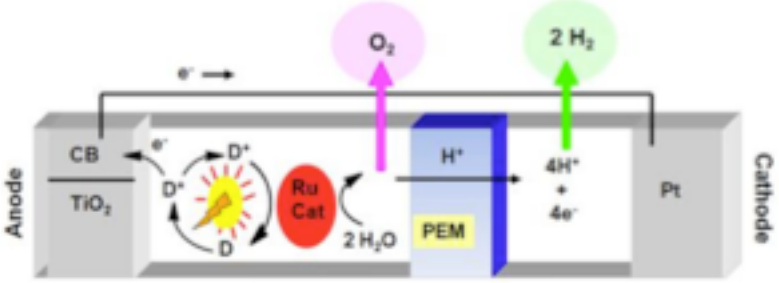
Molecular hydrogen is an attractive and clean energy vector. However, the question of where to get a sustainable hydrogen source remains unanswered. H_2 can be obtained from water splitting according to Eq. (1), a thermodynamically unfavoured process. Therefore, if sunlight wants to be used to overcome this trouble, a set of catalyzed redox half-reactions (Eq. (2) and (3)) should be coupled to a light-harvesting device in order to promote water splitting.

$$2H_2O \rightarrow 2H_2 + O_2 \qquad (1)$$

$$2\ H_2O \rightarrow O_2 + 4\ H^+ + 4\ e^- \qquad (2)$$

$$2\ H^+ + 2e^- \rightarrow H_2 \qquad (3)$$

Water oxidation (Eq. (2)) is nowadays the bottleneck reaction hampering the development of commercial devices for the photo-production of hydrogen as the one shown in Figure 1.



In the last seven years several Ru, Ir, Fe, Mn and Co molecular complexes which presents a relatively good performance with regards to this challenging reaction have been described, thoroughly characterized and mechanistically investigated.[1] The structure, catalytic performance and mechanistic details of some of these water oxidation systems will be discussed.

[1] (a) Sala, X.; Rodriguez, M.; Romero, I.; Escriche, L.; Llobet, A. *Angew. Chem. Int. Ed.* **2009**, *48,* 2842. (b) Romain, S.; Vigara, L.; Llobet, A. *Acc. Chem. Res*. **2009**, *42*, 1944-1953.