

Mechanism of water splitting catalyzed by the natural water-oxidizing catalyst

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A key step in natural photosynthesis is the water-splitting reaction into molecular oxygen, electrons and hydrogen equivalents. Understanding the molecular mechanisms behind this photoreaction will unravel the secrets of solar energy conversion in biochemistry and may inspire the design of artificial bio-mimetic materials for green energy production. Photosynthetic water oxidation occurs in the Mn_4Ca core of the Photosystem II complex where, through five subsequent steps, four electrons are sequentially removed until the oxidation of two water molecules. Here, using multiscale atomistic calculations, we investigated the molecular mechanism of the O_2 formation and release in Photosystem II^[1-4].

References

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