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A Hydrogen-Bond Stabilized Mechanism for Oxygen Evolution in Photosystem II: A Proposed Computational Experiment

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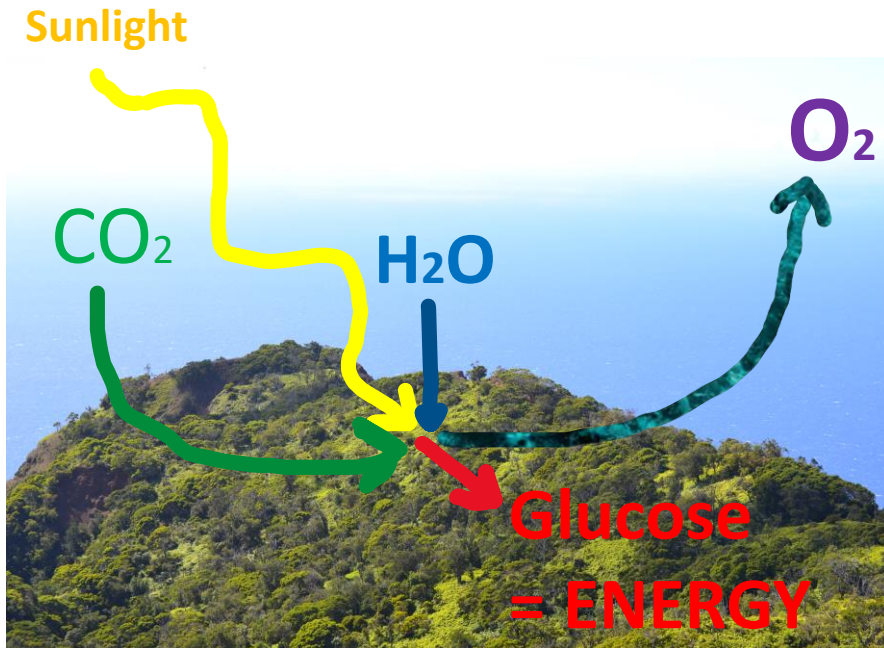
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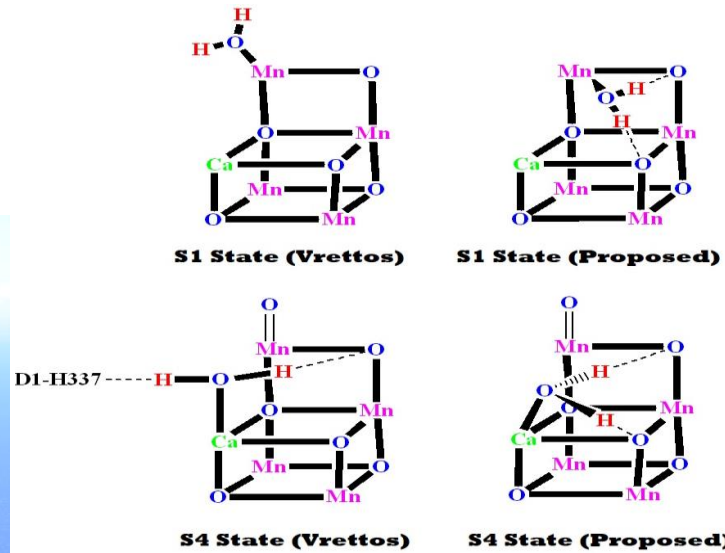
Faculty Mentor: Dr. Dong Wang, Department of Chemistry & Biochemistry, University of Montana

Oxygen Evolution at the OEC

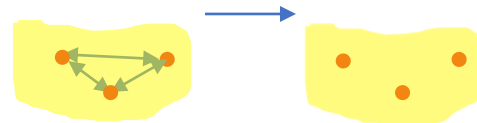


Okay, great...but at the molecular level, **no one knows exactly how this process works!**

This study identified a **key feature** of the OEC that may explain its activity.



Hohenberg-Kohn Theorem



Interacting fermions with real potential

Non-interacting fermions with effective potential...but same density!

Kohn's justification for DFT methods: all ground-state properties depend only on the electron density.

$$E(\rho) = E_{Kin}(\rho) + V_{eN}(\rho) + V_{ee}(\rho) + V_{xc}(\rho)$$

We can calculate all of these exactly...except V_{xc} .

Computational Details

The **lower energy structure is more likely to exist!**

*Comparative energy calculations arranged for Q-Chem 5.1 package DFT-D option (Dispersion-Corrected Density Functional Theory, D3 subset), using M06-L basis functionals. (Q-Chem inputs available in packet)

M06-L Exchange-Correlation Functionals:

$$E_x = \sum_{\sigma} \int [F_{X\sigma}^{PBE}(\rho_{\sigma}, \nabla\rho_{\sigma}) * f(w_{\sigma}) + \epsilon_{X\sigma}^{LSDA} h_X(x_{\sigma}, z_{\sigma})] dr$$

$$E_c = \int e_{\alpha\beta}^{UEG} [g_{\alpha\beta}(x_{\sigma}, x_{\sigma}) + h_{\alpha\beta}(x_{\alpha\beta}, z_{\alpha\beta})] dr$$

Does this actually matter?

- These results can be used to **guide new solar cell design.**
- One step closer to ***an alternative energy source whose only output is oxygen.***

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