Torque generation mechanism of ATP synthase\textsuperscript{1} JOHN MILLER, SLADJANA MARIC, M. SCOPPA, M. CHEUNG, University of Houston — ATP synthase is a rotary motor that produces adenosine triphosphate (ATP), the chemical currency of life. Our proposed electric field driven torque (EFT) model of FoF1-ATP synthase describes how torque, which scales with the number of c-ring proton binding sites, is generated by the proton motive force (pmf) across the mitochondrial inner membrane. When Fo is coupled to F1, the model predicts a critical pmf to drive ATP production. In order to fully understand how the electric field resulting from the pmf drives the c-ring to rotate, it is important to examine the charge distributions in the protonated c-ring and a-subunit containing the proton channels. Our calculations use a self-consistent field approach based on a refinement of reported structural data. The results reveal changes in pKa for key residues on the a-subunit and c-ring, as well as titration curves and protonation state energy diagrams. Health implications will be briefly discussed.

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John Miller
University of Houston

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