The Geochemical Signature of Biological Carbon Fixation

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Ribulose-1,5-bisphosphate carboxylase/oxygenase (RuBisCO), the predominant catalyst for the conversion of CO_2 to useful biomolecules, preferentially adds $^{12}CO_2$ over $^{13}CO_2$ during biological carbon fixation. This isotope fractionation creates a geochemical signal important to reconstructing past climate conditions and carbon cycling.[1] However, isotope fractionation is species-dependent, suggesting subtleties in the chemistry of RuBisCO's carbon fixation that have yet to be explored (Figure 1).

The path integral formulation of quantum mechanics provides approaches[2] to explore these subtleties by capturing the configurational sampling of the enzyme active site and the nuclear quantum effects of the reacting atoms (Figure 2). Here, we demonstrate the application of path integral approaches to biological carbon fixation and explore methods to achieve experimental accuracy through simulation.

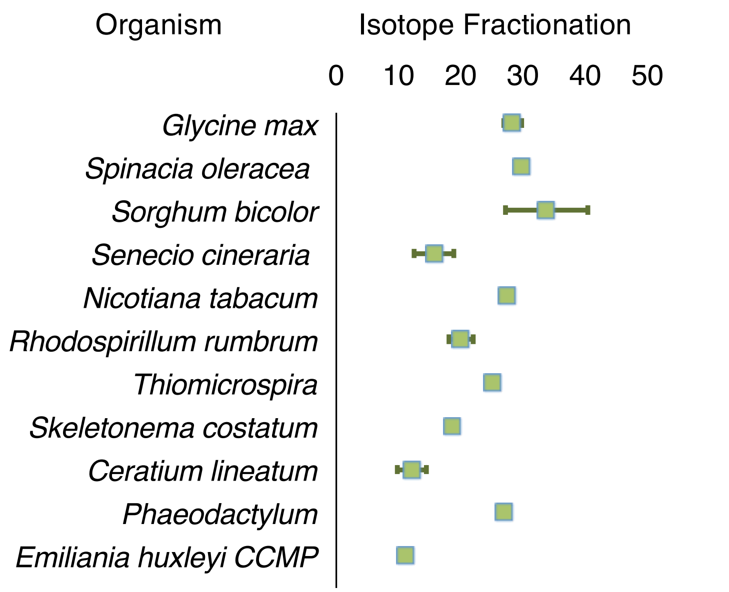

Figure 1: Carbon isotope fractionation in RuBisCOs from multiple species of autotrophs (see poster for full references).

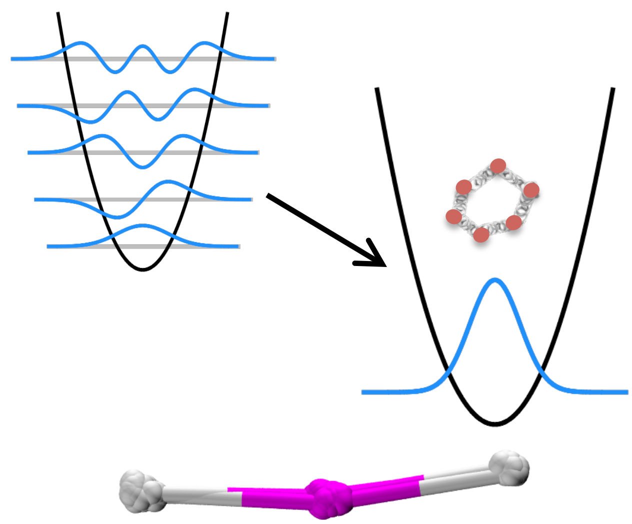

Figure 2: Top: Path integral approaches capture quantum Boltzmann statistics in a classical system. **Bottom:** A path integral model for CO_2.

1. Nisbet, E. G., et al. *Geobiology* 5.4 (2007): 311-35.
2. Chandler, D., Wolynes, P.G. *J. Chem. Phys.* 74 (1981): 4078-95.