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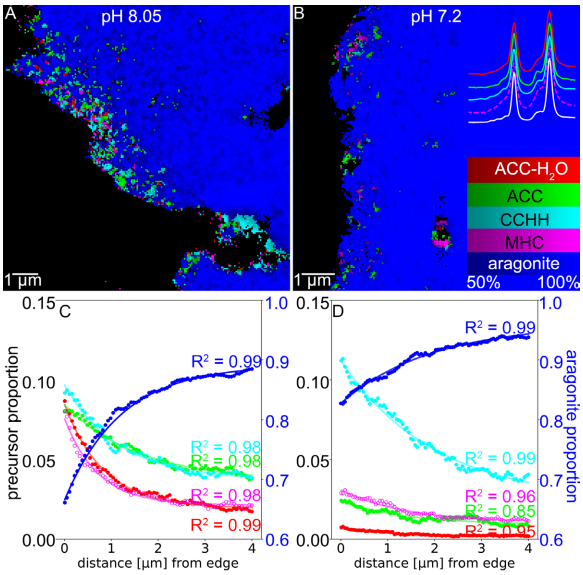
AI simulation-based inference to understand the dynamics of the animal-skeleton interface in corals

ZOË RECHAV[1] AND **PROF. PUPA GILBERT**[2,3]

[1]University of Wisconsin
[2]Lawrence Berkeley National Laboratory
[3]UW-Madison

It was previously revealed that there are four precursor phases to coral skeleton formation in diverse species, two amorphous and two crystalline, all transient, metastable, and occurring only on the surface in 50nm pixels (1). The forming surface is the animal skeleton interface in corals. More recently and in only one species, *Stylophora pistillata*, the proportions of these four precursors were found to decay exponentially, whereas the mature phase aragonite increased exponentially in the first 4 microns from the edge (2). These data are shown in Fig. 1. These exponential decays provide a unique, abundant (8 million pixels) and reliable testing ground to probe the kinetics of these mineral phases, including 8 variables (7 phase transitions between phases, and 1 nanoscale growth front velocity) using the artificial intelligence (AI) method termed simulation-based inference (SBI) (3). SBI was originally developed for particle physics, but it is extremely useful in many fields of science, because it uses simulations from any method to explore parameter spaces (e.g. the 8 above variables). Then, SBI matches the simulated outcomes to the data (e.g. the above exponential decays) to identify the most likely values for each parameter. If SBI works for coral skeletons, it will produce the first quantitative energy landscape including all phases and phase transitions' activation barriers for aragonite biomineralization (Fig. 2).

1. CA Schmidt et al. *Nat Commun* (2024) DOI: https://doi.org/10.1038/s41467-024-46117-x.
2. Z Rechav et al. *Nat Commun* (2026) DOI: https://doi.org/10.1038/s41467-026-69215-4
3. K Cranmer et al. PNAS (2020) DOI: https://doi.org/10.1073/pnas.1912789117



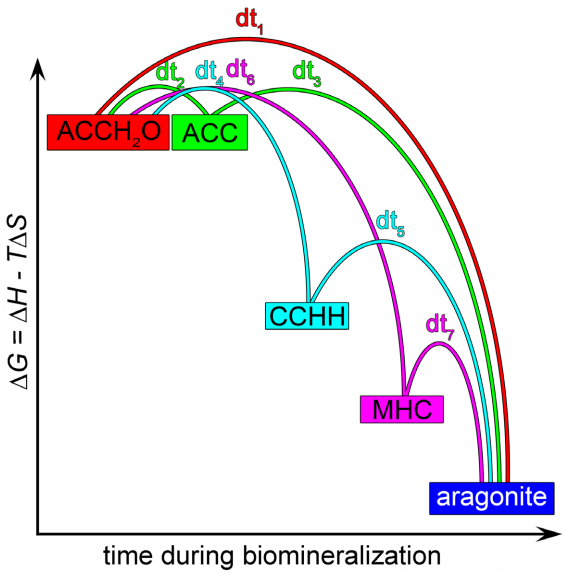


Figure 1. Exponential decays (data from ref 2). Figure 2. Energy landscape (adapted from ref 1).