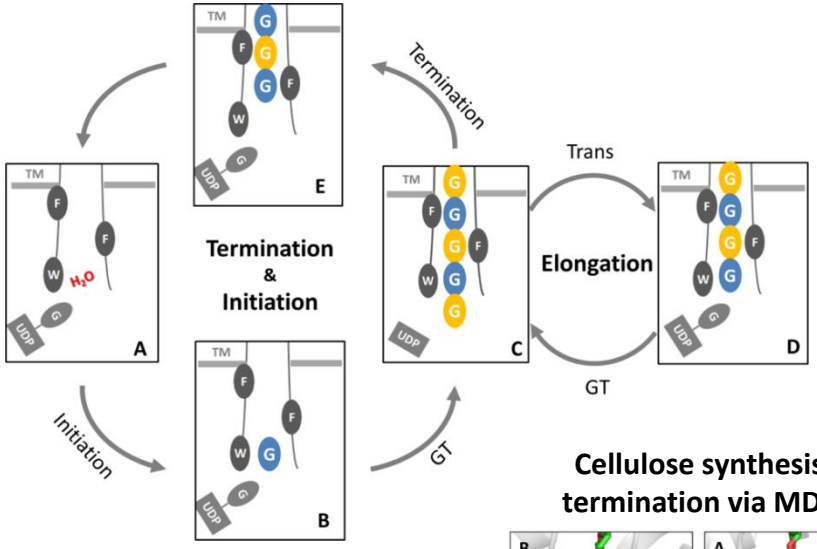
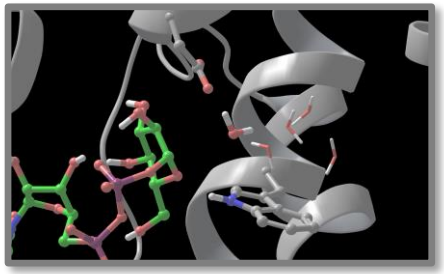
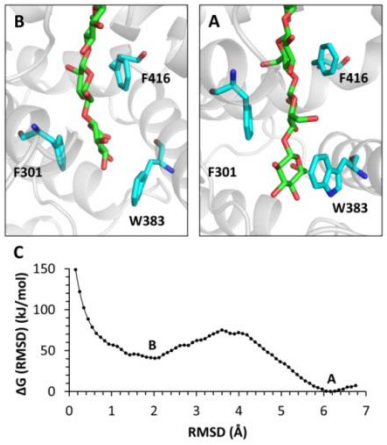
Chain Initiation and Termination by Cellulose Synthase



Cellulose synthesis initiation based on QM/MM calculations.



Cellulose synthesis termination via MDS



Yang, H.; McManus, J. B.; Oehme, D.; Singh, A.; Yingling, Y. G.; Tien, M.; Kubicki, J. D. Simulations of Cellulose Synthesis Initiation and Termination in Bacteria *The Journal of Physical Chemistry B* 2019, 123, 17, 3699-3705. [w/Cover image]

Significance and Impact

This study provides detailed insights into how a cellulose chain can be synthesized without a primer by cellulose synthase, and how the degree of polymerization (DOP) of the cellulose chain is controlled by the transmembrane (TM) tunnel of the enzyme. This work suggest ways to genetically engineer the enzyme to produce cellulose of favorable chain lengths for biofuel and material uses.

Scientific Results

- **H_2O molecules can break down UDP-glucose to start a new cellulose chain;**
- **Termination of cellulose synthesis is associated with one extra step of chain translocation;**
- **The DOP is related to the affinity of the cellulose chain to the TM tunnel of the enzyme. Decreasing cellulose affinity to the TM tunnel reduces DOP.**

Research Details

Using MD simulations and QM/MM calculations of BcsA, a cellulose synthase from *Rhodobacter sphaeroides*, we detail the molecular mechanisms of cellulose chain initiation, elongation and termination.

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