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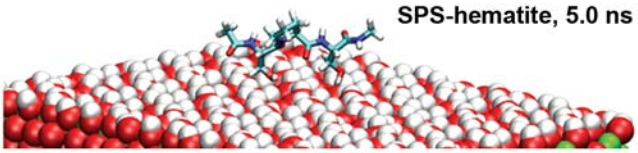
EMSL Science Made Possible

The peptide that binds

Fundamental mechanisms of mineral-microbe interactions illuminated

A diverse team of geologists, biologists, and computer scientists from the Pacific Northwest National Laboratory, The Ohio State University, and Virginia Tech is looking into how microorganisms bind to iron oxide. These interactions, common in the subsurface, are of importance to understanding the transport of environmental contaminants and subsequent remediation. Using computational and experimental resources at the Department of Energy's EMSL, the team found the protein fragment or polypeptide, just 9 amino acids long, that glues the larger protein to iron oxide.



Snapshot of the SPS-hematite simulation at 5.0 ns. *The peptide adopts a conformation that allows its two serine residues to form hydrogen bonds with hematite and template the iron oxide surface.*

To find this binding polypeptide, the team began with phage technology, using a virus to create more than 3 billion different polypeptides. They screened these molecules and found the polypeptide that would bind to hematite. Next, they performed molecular simulations using an AMBER96 force field with EMSL's NWChem. The simulations showed that the polypeptide takes on a shape that matches the mineral surface, allowing it to grip the surface. Finally, the team searched the genomes of numerous bacteria to see if the polypeptide existed in microbes known for their interactions with metal oxides and found the sequence in *Thalassiosira pseudomona* and *Shewanella oneidensis*.

Scientific impact: This research answers a fundamental question in polypeptide binding and could aid researchers in everything from better understanding geochemical processes to designing and controlling material synthesis for biofuel cells. This work is part of EMSL's continued effort to link theory and simulations to experiments in real time.

Societal impact: The peptide binding data provides insights into geochemistry that may be of value to subsurface cleanup. In addition, by identifying the polypeptide that binds the protein to the iron, researchers are a step closer to designing biobased fuel cells, which could replace certain fossil fuels while producing fewer pollutants.

For more information, contact EMSL Communications Manager Mary Ann Showalter (509-371-6017).

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User Proposals 19842 and 9593