

# Special Bio-Inorganic Chemistry **Seminar**

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## “ Structural Evidence for Dynamic Nitrogenase Metallocluster ”

**Abstract:** Nitrogenase catalyzes dinitrogen reduction to ammonia and is the only enzyme capable of supplying the world with a reduced form of 'N' that can be directly incorporated into biomolecules such as DNA and proteins. The most well-studied nitrogenase, molybdenum nitrogenase, consists of two component proteins, the Fe protein (a homodimer with a 4Fe4S cluster) and the MoFe protein (a heterotetramer with two complex metalloclusters per heterodimer). During catalysis, the two proteins associate, allowing ATP-dependent electron transfer from the Fe protein to the MoFe protein. In the as-isolated state, the MoFe protein active site (FeMo-cofactor) has an overall composition of [7Fe:9S:1C:1Mo]-R-homocitrate. This form of the FeMo-cofactor does not bind substrate and requires activation (by the Fe protein) prior to substrate binding. As a result, only recently have ligand bound states of the protein bound FeMo-cofactor been crystallographically determined. Selenium can function as a sulfur-surrogate, exchanging with labile sulfide groups under various conditions, resulting in Se-incorporated metalloclusters. In my talk, I will present crystallographic evidence for Se-incorporation into the nitrogenase metalloclusters and discuss the mechanistic implications of these findings.

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**4:00 p.m. | Via Zoom**

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