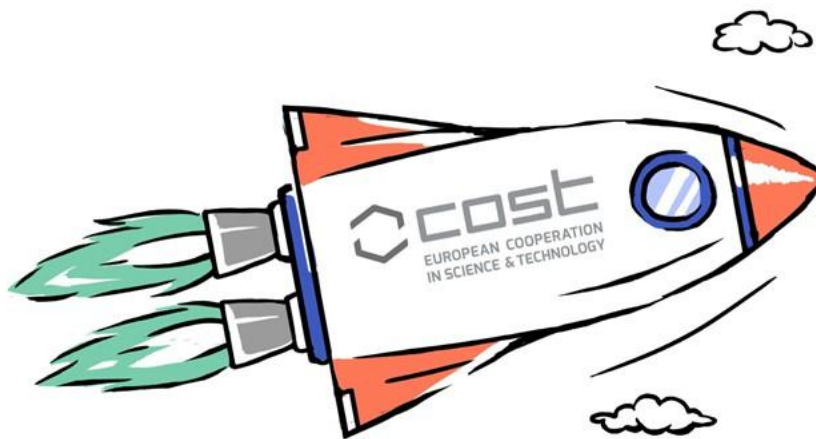




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WG4. Mechanistic studies of FeS chemistry

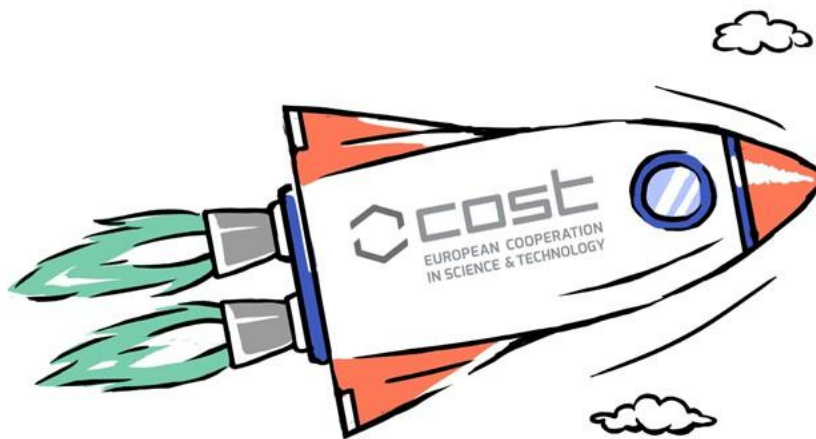
Deliverables

Deliverable 15. Report on intermediates of catalytic function of FeS enzymes like members of radical-SAM enzymes (RSAD1 and RSAD2).

Deliverable 16. Report on the reaction of FeS clusters with nitric oxide, hydrogen peroxide, and dioxygen.

Deliverable 17. Scientific papers on protocols for overexpression of FeS enzymes and mechanistic studies of FeS chemistry.

Period: Nov 2022 – Nov 2026



Deliverable 15-16

Executive Summary

Working Group 4 (WG4) has delivered transformative insights into the fundamental chemistry of iron-sulfur (Fe-S) clusters, spanning from gasotransmitter sensing and oxidative stress responses to catalytic mechanisms in complex metalloenzymes. The outputs from this reporting period represent a comprehensive integration of computational chemistry, synthetic model systems, advanced spectroscopy, and mechanistic enzymology. Key achievements include: (1) elucidation of the complete electron transfer landscape in [FeFe]-hydrogenase catalytic mechanism; (2) establishment of mitoNEET as a bona fide O_2/NO gas sensor with implications for hypoxia signaling; (3) systematic dissection of first- and second-sphere interactions in synthetic Fe_4S_4 clusters; (4) structural and functional characterization of the ancestral SMS Fe-S biogenesis system; (5) discovery of a conserved tripeptide motif governing client recognition in eukaryotic Fe-S cluster delivery; (6) detailed mechanistic insights into NO-mediated regulation of the NsrR transcription factor; and (7) characterization of redox-dependent stability in C1SD3 and metal homeostasis in pathogenic fungi. These findings collectively advance our understanding of Fe-S cluster reactivity with small molecules (NO , H_2O_2 , O_2) and establish new paradigms for catalytic function and biological regulation.

1. Reactions of FeS Clusters with Nitric Oxide, Hydrogen Peroxide, and Dioxygen

1.1. MitoNEET as an O_2/NO Gas Sensor (Outputs 4 & 5)

The mitochondrial outer membrane protein mitoNEET has long been studied as a drug target and metabolic regulator, but its molecular function remained elusive. WG4 has now established a paradigm-shifting model for mitoNEET function in gasotransmitter sensing.

- **Finding:** An interdisciplinary approach combining structural analysis, computational modeling, and biochemical characterization revealed an **explicit nitric oxide (NO) access site** to the mitoNEET [2Fe-2S] cluster.
- **O₂ Protection Mechanism:** Molecular oxygen (O₂) and the anti-diabetic drug pioglitazone **physically block NO access** to the cluster. This discovery suggests that the mitoNEET [2Fe-2S] cluster functions as a **cellular O₂ sensor**, where:
 - Under **normoxia**, O₂ binds/protects the cluster, preventing NO attack.
 - Under **hypoxia**, O₂ dissociates, exposing the cluster to NO and triggering downstream signaling.
- **Biological Implications:** This mechanism explains how mitochondria sense hypoxia and modulate bioelectrochemistry, fission/fusion dynamics, and mitophagy. The findings link Fe-S cluster chemistry to age-related neurodegeneration and immune dysfunction.
- **Action Impact:** This represents a **new paradigm in Fe-S biology**—clusters as dynamic gas sensors rather than static electron transfer cofactors. The work opens therapeutic avenues for inflammatory and age-related diseases by targeting the mitoNEET O₂/NO sensing axis.

1.2. CISD3 Redox Stability and Differential Sensitivity to H₂O₂ and NO (Output 9)

Among the human NEET proteins, CISD3 has been the least characterized. WG4 has now provided comprehensive biochemical and cellular insights into its redox chemistry and stress responses.

- **Finding:** CISD3 exists predominantly in the **reduced form** in cells, displaying a single sharp voltammetric signal at −31 mV vs. SHE, suggesting cooperative electron transfer between its two [2Fe-2S] clusters.
- **Differential Stress Sensitivity:**
 - **Iron deficiency:** CISD3 loses its Fe-S clusters, becomes unstructured, and undergoes drastic cellular degradation.
 - **Hydrogen peroxide (H₂O₂):** The oxidized form of CISD3 is particularly sensitive to H₂O₂ in vitro; however, in cellulo, CISD3 is **unaffected by H₂O₂-induced oxidative stress**, likely due to its predominant reduced state.
 - **Nitric oxide (NO):** Only the reduced form of CISD3 binds NO. Paramagnetic NMR revealed that NO binding triggers **cluster disassembly while iron ions remain protein-bound**. In cellulo, CISD3 becomes highly unstable upon NO treatment.
- **Mechanistic Insight:** Chemical shift perturbation studies revealed a **redox-associated conformational change at the C-terminal CDGSH domain** that determines the instability of the oxidized state and may underlie cooperative electron transfer.
- **Action Impact:** These findings establish CISD3 as a redox sensor with distinct responses to different gasotransmitters, providing a framework for understanding its role in cancer, diabetes, and neurodegeneration.

1.3. NsrR: Exquisite NO Sensitivity in Transcriptional Regulation (Output 11)

The Rrf2 family protein NsrR is a key regulator of nitrosative stress responses in bacteria, but the precise point at which NO binding abolishes DNA binding was unknown. WG4 has now quantified this critical regulatory threshold.

- **Finding:** Using surface plasmon resonance (SPR) and native mass spectrometry (MS), the study demonstrated that:
 - **Holo NsrR** (two [4Fe-4S] clusters per dimer) binds promoter DNA with nanomolar affinity.
 - **Hemi-apo NsrR** (one cluster per dimer) binds >10-fold less tightly.
 - **Apo NsrR** (no clusters) does not bind DNA at all.
 - **Critical Discovery:** Reaction of DNA-bound NsrR with **a single NO molecule per dimer is sufficient to abolish DNA binding**. This exquisite sensitivity ensures rapid de-repression of NO detoxification genes at the earliest opportunity.
 - **Physiological Relevance:** Previously characterized iron-nitrosyl species formed at higher NO:cluster ratios are **not physiologically relevant** for the NsrR on/off switch. The regulatory mechanism operates through a minimal NO signal that triggers cluster modification and DNA release.
 - **Action Impact:** This work establishes NsrR as one of the most sensitive NO sensors known and provides a quantitative framework for understanding bacterial responses to nitrosative stress from host immune systems.
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2. Intermediates of Catalytic Function in FeS Enzymes

2.1. Complete Electron Transfer Landscape in [FeFe]-Hydrogenase (Output 1)

[FeFe]-hydrogenases are among the most efficient biological catalysts for H₂ production/oxidation, yet the role of accessory Fe-S clusters in the catalytic mechanism has remained incompletely understood. WG4 has now provided a comprehensive computational analysis.

- **Methodology:** Hybrid quantum mechanics/molecular mechanics (QM/MM) methods were employed to characterize the electronic structure and thermodynamic landscape of redox and protonation events across the **complete Fe-S cluster network** of *Desulfovibrio desulfuricans* hydrogenase (DdHydAB), including the [4Fe-4S]H subcluster, the [2Fe]H organometallic unit, and accessory F and F' clusters.
- **Key Findings:**
 - The **F' cluster** is the **preferential site for the first electron** during reduction of the oxidized resting state, acting as an electron reservoir.

- Strong coupling between **protonation and electron transfer (PCET)** was identified: protonation at the H-cluster induces electron transfer from F' to the H-cluster.
- Formation of a **terminal hydride** is energetically favored over protonation of the azadithiolate (ADT) ligand.
- Subsequent **isomerization to a bridging hydride (μ -H)** provides further stabilization but may be kinetically limiting.
- **Action Impact:** This study demonstrates that the catalytic mechanism of [FeFe]-hydrogenases cannot be understood by considering the H-cluster in isolation; the entire Fe-S cluster network participates in electron distribution and redox poising, with PCET coupling as a central feature.

2.2. Rational Engineering of [FeFe]-Hydrogenase Maturation (Output 2)

Building on mechanistic understanding of [FeFe]-hydrogenase structure, WG4 has addressed a critical bottleneck in the industrial application of these biocatalysts.

- **Finding:** The slow in vitro maturation of DdHydAB apo-enzyme with synthetic cofactor mimics was attributed to **inefficient rearrangement of a critical "locking element"** near the active site after cofactor uptake.
- **Engineering Solution:** Subunit fusion with short peptide linkers was employed to facilitate the required conformational change.
- **Outcome:** The modification increased the **maturation rate by up to 41-fold** without compromising catalytic performance.
- **Mechanistic Contribution:** The findings elucidate a key step in the **"plug-lock-lid" mechanism** of [FeFe]-hydrogenase maturation, providing a general framework for engineering metalloenzyme maturation pathways.
- **Action Impact:** This work advances the scalable production of holo-[FeFe]-hydrogenases, promoting their industrial applicability for sustainable H₂ production and oxidation.

2.3. First- and Second-Sphere Interactions in Fe₄S₄ Clusters (Output 3)

Understanding how protein environments tune Fe-S cluster properties is fundamental to mechanistic enzymology, yet disentangling covalent from noncovalent effects has remained challenging. WG4 has now provided a systematic analysis using synthetic model complexes.

- **Methodology:** A series of synthetic Fe₄S₄ complexes was designed to independently assess **first-sphere (covalent) interactions** (e.g., histidine ligation) and **second-sphere (electrostatic/dipolar) interactions**.
- **Key Findings:**
 - First-sphere interactions **"fine-tune" the electronic/magnetic structure** of [Fe₄S₄]¹⁺/²⁺/³⁺ complexes in a manner that **persists at ambient temperatures**.

- Second-sphere electric dipolar interactions produce observable effects at extremely low temperatures but do **not significantly alter the clusters' gross electronic/magnetic structure at temperatures relevant to enzyme function.**
- **Energetic Distinction:** The study establishes a **clear energetic hierarchy**: first-sphere covalent interactions dominate the functional properties of Fe-S clusters under physiological conditions, while second-sphere electrostatic effects are comparatively minor.
- **Action Impact:** These results provide a critical framework for interpreting spectroscopic data from biological systems, facilitating identification of functionally relevant protein-cofactor interactions and strengthening our understanding of structure-function relationships in Fe₄S₄ cofactors.

2.4. ATP-Dependent Fe(CN)₂CO Transfer in [NiFe]-Hydrogenase Maturation (Output 10)

The maturation of [NiFe]-hydrogenases requires the HypCD complex to assemble and transfer the Fe(CN)₂CO subfragment, but the role of its ATPase activity has remained mysterious. WG4 has now uncovered unexpected mechanistic details.

- **Finding:** Comprehensive spectroscopic characterization using infrared, Mössbauer, and nuclear resonance vibrational spectroscopy (NRVS) revealed **molecular details of Fe(CN)₂CO coordination** to the HypCD complex.
- **ATP Requirement Deciphered:** Combining biochemical assays, spectroscopy, AlphaFold structure predictions, protein-ligand docking, and crosslinking MS revealed that **ATP hydrolysis triggers the transfer of the Fe(CN)₂CO fragment** to the apo-hydrogenase subunit.
- **Mechanistic Insight:** The ATPase activity of HypCD does not function in cluster assembly per se but rather in **driving the conformational change or energetically unfavorable transfer step** required for cofactor delivery.
- **Action Impact:** This work resolves a long-standing mechanistic question in [NiFe]-hydrogenase maturation and establishes a general principle for ATP-dependent cofactor transfer in metalloenzyme biogenesis.

2.5. The SMS System: An Ancestral Fe-S Biogenesis Machinery (Output 6)

Understanding the evolutionary origins of Fe-S biogenesis provides insights into fundamental chemical principles. WG4 has characterized the ancestral SMS system from the hyperthermophilic archaeon *Methanocaldococcus jannaschii*.

- **Finding:** The SMS system forms a **SmsC₂B₂ heterotetramer** wherein the SmsC subunit hosts both ATP and [Fe-S] cluster binding sites.
- **Regulatory Coupling:** ATP binding and [Fe-S] cluster assembly are **mutually exclusive**, allowing for regulatory coupling between substrate binding events.

- **Cluster Assembly and Transfer:** Mutagenesis identified key Cys residues in SmsC required for cluster assembly. The SMS system **rescued a non-viable *E. coli* strain lacking ISC and SUF systems** under anoxic conditions with Na₂S as sulfur source.
- **Evolutionary Model:** The study proposes that SMS represents an ancestral system dating to the Last Universal Common Ancestor, which operated in anaerobic prokaryotes before evolving into the SUF system following the Great Oxidation Event.
- **Action Impact:** This work establishes SMS as a new bona fide Fe-S biogenesis system and provides evolutionary context for understanding how Fe-S chemistry adapted to the transition from an anoxic to an oxic world.

2.6. Client Recognition in Eukaryotic Fe-S Cluster Delivery (Output 12)

The eukaryotic cytosolic iron-sulfur protein assembly (CIA) pathway must deliver clusters to >30 different client proteins, raising fundamental questions about specificity. WG4 has now identified the molecular determinant.

- **Finding:** A conserved **tripeptide motif [LIM]-[DES]-[WF]-COO⁻** at the C-terminus is present in more than a quarter of CIA clients or their adaptors.
- **Functional Validation:** This **targeting complex recognition (TCR) motif** is **necessary and sufficient** for:
 - Binding to the CIA-targeting complex (CTC) in vitro.
 - Directing Fe-S cluster delivery in vivo.
- **Bioengineering Application:** Fusion of the TCR signal to a nonnative protein **enabled engineering of cluster maturation** via recruitment of the CIA machinery.
- **Action Impact:** This discovery provides fundamental insights into the biochemistry of Fe-S protein maturation and unlocks the potential for bioengineering Fe-S cluster delivery to nonnative enzymes—a critical bottleneck in synthetic biology applications.

3. Additional Contributions: Metal Homeostasis in Pathogenic Fungi

3.1. Ferroportin Homolog FpnA in *Aspergillus fumigatus* (Output 7)

While not directly focused on Fe-S chemistry, this output contributes to WG4's broader understanding of iron homeostasis and its relationship to Fe-S biogenesis in pathogenic organisms.

- **Finding:** The *A. fumigatus* ferroportin homolog **FpnA** is localized to the **vacuolar membrane** and mediates resistance to nickel, cobalt, and gallium—not iron.
- **Mechanistic Insight:** FpnA functions in **detoxification by vacuolar deposition** of substrate metals, rather than iron efflux as in vertebrates.

- **Evolutionary Significance:** The divergent localization and function of ferroportin homologs between metazoa and fungi highlights the plasticity of metal homeostasis systems.
- **Action Impact:** This work underscores the importance of understanding metal homeostasis in pathogenic fungi as a potential therapeutic target and provides evolutionary context for the diversification of iron/metal transport systems.

3.2. HapX: [2Fe-2S] Cluster-Mediated Iron Sensing in Fungal Virulence (Output 8)

The transcription factor HapX is crucial for *A. fumigatus* virulence, but how it senses and responds to varying iron availability was unknown. WG4 has now revealed a cluster-based sensing mechanism.

- **Finding:** HapX contains **four conserved cysteine-rich regions (CRRs)** with different propensities to coordinate [2Fe-2S] clusters, resulting in **cumulative occupancies depending on iron availability**:
 - **Iron starvation:** No clusters in any CRR.
 - **Iron sufficiency ("neutral" state):** Clusters in CRR-B and/or CRR-C.
 - **Iron excess:** Clusters in CRR-A, -B, and -C (CRR-D plays a minor role).
 - **Functional Consequences:** Combinatorial mutation of CRR-B and -C locked HapX in the iron starvation state, causing **uncontrolled iron uptake** and repression of iron-consuming pathways and detoxification.
 - **Additional Discovery:** The HapX iron starvation state induced several **gene clusters encoding secondary metabolites**, suggesting a link between iron sensing and secondary metabolism.
 - **Action Impact:** This study establishes HapX as a **three-state iron sensor** regulated by differential [2Fe-2S] cluster occupancy, providing a mechanistic model for how fungi adapt to varying iron availability during infection.
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4. Synthesis and Future Directions for WG4

The outputs from this reporting period establish WG4 as a leader in mechanistic Fe-S chemistry, spanning from fundamental reactivity to biological regulation.

Key Mechanistic Themes:

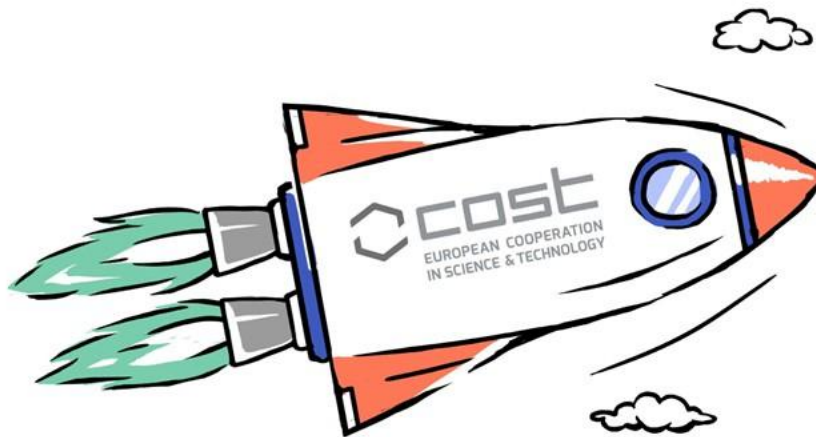
1. **Fe-S Clusters as Gas Sensors:** The mitoNEET O₂/NO sensing mechanism, CISD3 differential stress responses, and NsrR NO sensitivity collectively establish that Fe-S clusters can function as **exquisite sensors of gaseous signaling molecules** with physiological relevance.
2. **Electron Transfer Networks in Catalysis:** The [FeFe]-hydrogenase QM/MM study demonstrates that catalytic function requires understanding the **entire Fe-S cluster network**, not just the active site.

3. **Conformational Dynamics in Maturation:** The hydrogenase maturation engineering and ATP-dependent $\text{Fe}(\text{CN})_2\text{CO}$ transfer studies highlight the importance of **protein conformational changes** in cofactor delivery.
4. **Molecular Recognition in Cluster Delivery:** The TCR motif discovery and SMS structural characterization reveal that **specific recognition determinants** govern cluster assembly and transfer across evolutionarily diverse systems.
5. **Evolutionary Adaptation to Oxygen:** The SMS system characterization provides insight into how Fe-S chemistry evolved from anaerobic to aerobic environments.

Proposed Next Steps for WG4:

1. **Time-Resolved Spectroscopy of NO Reactions:** Following the NsrR and CISD3 studies, WG4 will pursue time-resolved spectroscopic approaches (stopped-flow UV-vis, rapid-freeze EPR, time-resolved Mössbauer) to capture intermediates in the reaction of Fe-S clusters with NO.
2. **Expanding the mitoNEET Sensing Paradigm:** WG4 will investigate whether other NEET proteins (CISD1, CISD2) exhibit similar O_2/NO sensing capabilities and map the complete signal transduction pathways downstream of cluster modification.
3. **PCET in Fe-S Enzymes:** Building on the [FeFe]-hydrogenase findings, WG4 will systematically investigate proton-coupled electron transfer in other Fe-S enzymes, including aconitase, ferredoxins, and radical-SAM enzymes.
4. **Bioengineering Fe-S Enzymes:** The TCR motif discovery will be leveraged to engineer novel Fe-S enzymes for synthetic biology applications, with initial focus on nonnative hydrogenase and nitrogenase expression in eukaryotic systems.
5. **Cross-WG Collaboration:** WG4 will collaborate with WP2 and WP3 to apply mechanistic insights from SMS and SUF systems toward developing antimicrobial strategies targeting Fe-S biogenesis in pathogens.

Disclaimer: *This report is a synthesis document prepared for COST Action Working Group 4 based on the provided abstracts. Specific grant numbers and author lists are omitted for brevity but are available in the original publications.*



Deliverable 17

Publications

1. QM/MM Modeling of the Electronic Structure and Properties of the Fe–S Clusters in *Desulfovibrio desulfuricans* [FeFe]-Hydrogenase, *Inorg Chem.* (2026) 65(25):13988–13999. DOI: [10.1021/acs.inorgchem.6c01252](https://doi.org/10.1021/acs.inorgchem.6c01252)
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5. Discovery of an Antiviral Electron Transfer Process to Create Catalytically Self-Sufficient Viral Restriction Factors, *Angewandte Chemie* (2026), e5423408. DOI: <https://doi.org/10.1002/anie.5423408>
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