Volendo semplificare.

1. Ho creato/adattato un database termodinamico (Calphad) che comprende i carburi metastabili epsilon, eta, chi ed Fe7C3 ( oltre alla Fe3C naturalmente)

|  |
| --- |
|  |
| Figura 1 Database termodinamico per i carburi epsilon, eta, chi |

|  |
| --- |
|  |
| Figura 2 Un diagramma di stato dal “mio” database termodinamico con i carburi epsilon e Fe7C3 |

|  |
| --- |
|  |
| Figura 3 Un diagramma di stato dal “mio” database termodinamico con i carburi eta, chi (Fe5C2) e Fe7C3 con l’ esclusione della cementite Fe3C |

1. Ho iniziato a produrre dei semplicissimi programmi di calcolo del campo iperfine dei carburi di ferro (in Matlab/Octave) che possano rendere piu' significativo il fitting delle diverse fasi dei  diversi "iron environments" basandomi principalmente sul lavoro di Paalanen, Utrecht University

|  |
| --- |
|  |
| Figura 4a Una figura dal “mio” programma per la semplice simulazione con distribuzione di campo iperfine di carburi epsilon, eta, chi, theta e theta Fe7C3 di macinazione di cementite con mulino Spex 8000 per 7.5 h ( BPR 20:1) |
|  |
| Figura 4b Una figura dal “mio” programma: stesso campione, distribuzione di campo iperfine di carburi con il confronto tra la “mia” distribuzione e quella calcolata da un programma Fortran “professionale” |

1. Per la diffrazione di raggi X e la  spettroscopia Mossbauer (che pure avevamo qui ad Udine, ma diversi anni fa sono state rottamate perfettamente funzionanti)  collaboro attivamente con l' Universita' di Olomouc  e con il suo  spin-off Iron Analytics, avendo la possibilita' di lavorare anche in CEMS

|  |
| --- |
|  |
| Figura 5 Diffrattogramma di acciaio 100 Cr 6 – Sample S1 ricevuta da Olomouc questo mese |

|  |
| --- |
|  |
| Figura 6 Diffrattogramma di acciaio 100 Cr 6 – Sample S1 ricevuta da Olomouc questo mese confrontai con miei antichi dati diffrattometrici |

|  |
| --- |
|  |
|  |

|  |  |
| --- | --- |
|  |  |
|  |  |

|  |
| --- |
|  |
|  |
|  |

**Interdisciplinary Research Project Proposal: Fundamental Properties and Applications of Iron Carbides**

**Project Duration: 3 years**

**Coordinator: Fabio Miani**

**1. Project Overview**

This interdisciplinary research project aims to comprehensively investigate the fundamental properties and diverse applications of Iron Carbides. By bringing together experts from various fields and utilizing cutting-edge techniques, we seek to advance our understanding of Iron Carbides and explore their potential in multiple sectors.

**2. Research Sectors and Team Members**

1. **Physics: Density Functional Theory Applied to Iron Carbides**
   * Lead: Stefano Curtarolo
2. **CALPHAD (CALculation of PHAse Diagrams)**
   * Team: Zi-Kui Liu, Bengt Hallstedt, Aurelie Jacob, Erwin Povoden-Karadenic, Bo Sundman, Taichi Abe
3. **Mechanochemical Synthesis and Mössbauer Characterization of Iron Carbides**
   * Lead: Francesco Delogu
4. **Iron Carbides in Earth's Inner Core**
   * Lead: Eli Brosh
5. **Use of Iron Carbides in Fischer-Tropsch Process**
   * Team: Xiao-Dong Wen, Esna Du Plessis, Pasi Paalanen
6. **Iron Carbides and Bainite**
   * Lead: H.D.K.H. Bhadeshia
7. **Iron Carbides and DRI (Direct Reduced Iron) Process**
   * Team: Alessandro Martinis, Stefano Maggiolino
8. **Synchrotron Radiation for Iron Carbides Characterization**
   * Team: Marco Peloi, Catherine McCammon, Clemens Prescher
9. **Development of Disruptive Bainitic Steels**
   * Team: Francesca Maurigh, Cristophe Stocky

**3. Research Objectives**

1. Develop accurate theoretical models of Iron Carbides using density functional theory.
2. Improve CALPHAD databases and models for Iron-Carbon systems.
3. Optimize mechanochemical synthesis methods for Iron Carbides.
4. Enhance understanding of Iron Carbides' role in Earth's inner core.
5. Improve Fischer-Tropsch processes using Iron Carbide catalysts.
6. Advance the understanding of Iron Carbides in bainitic transformations.
7. Optimize the DRI process through better control of Iron Carbide formation.
8. Develop new characterization techniques using synchrotron radiation.
9. Design and develop novel bainitic steels with precisely controlled Iron Carbide structures.

**4. Methodology**

Each research sector will employ specific methodologies relevant to their field. Some key approaches include:

* Computational modeling and simulation
* Advanced material synthesis techniques
* Cutting-edge characterization methods (e.g., Mössbauer spectroscopy, synchrotron radiation)
* Experimental studies of material properties and performance
* Process optimization and scale-up studies

**5. PhD Student Involvement**

We propose involving six PhD students, each focusing on a specific aspect of the project:

1. Computational modeling of Iron Carbides
2. CALPHAD modeling of Fe-C systems
3. Mechanochemical synthesis and characterization of Iron Carbides
4. Iron Carbides in geophysical contexts
5. Catalytic applications of Iron Carbides
6. Iron Carbides in steel metallurgy

**6. Expected Outcomes**

1. Advanced theoretical models for Iron Carbides
2. Improved CALPHAD databases for Fe-C systems
3. Novel synthesis methods for Iron Carbides
4. Better understanding of Earth's inner core composition
5. Enhanced Fischer-Tropsch catalysts
6. Improved bainitic steel designs
7. Optimized DRI processes
8. New characterization techniques for Iron Carbides
9. Prototype disruptive bainitic steels

**7. Dissemination Plan**

* Regular consortium meetings and workshops
* Publications in high-impact peer-reviewed journals
* Presentations at international conferences
* Development of a project website and social media presence
* Engagement with industry partners for potential commercialization

**8. Timeline**

* Year 1: Establish theoretical frameworks, initiate experimental work
* Year 2: Continue experiments, begin integrating results across disciplines
* Year 3: Finalize experiments, focus on applications and prototyping

**9. Budget Considerations**

(To be developed in consultation with all team members and institutional requirements)

**10. Potential Funding Source**

Big Ticket RFCS (Research Fund for Coal and Steel) project

**11. Next Steps**

1. Review and refine this draft proposal with all team members
2. Consult with Alessandra Colli (EU officer) for pre-projectual advice
3. Prepare final proposal for submission by April 2025

|  |  |
| --- | --- |
|  |  |
|  |  |