# Hao (Charles) Chen

M.Sc

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## Research Interests

Phase Transitions in Materials
Materials Simulation in Real Thermodynamic Conditions
Machine Learning in Materials Science

## Education

**Master** in Materials Science and Engineering **2021**
Tongji University (985/211 national key univ, QS Ranking: 211) Shanghai, China
GPA: 4.19/5 Average Score: 84.48/100

**Bachelor** in Materials Science and Engineering **2017**
Hebei University of Science & Technology Hebei, China
GPA: 3.51/4 Average Score: 85.66/100

## Professional Skills

**Language:** Chinese Mandarin (native), English (CET-6 score:525)
**Scientific Software:** CASTEP, VASP, VTST, Materials Studio, CrystalMaker, VESTA
**Operate System:** Windows, Linux
**Characterization:** XRD, TEM, SEM, AFM, OES
**Computing:** Machine Learning, Python (both with Coursera certificates)

## Dissertation

**"First-principles investigation of the evolution mechanism of ω phase and carbides in Fe-C alloys"**

Supervisor: Prof. Hongping Xiang

Methods: Simulation (VASP, CASTEP) and Experiment (XRD, TEM, SEM)

- Confirmed the existence of ω-Fe phase which has been neglected for decades in carbon steel and iron-carbon diagram.
- Proposed the stability mechanism of ω-Fe phase and its relationships with α-Fe and γ-Fe.
- Suggested a new formation process of cementite (θ-$Fe_3C$) and pearlite which are key factors for steel properties.

## Teaching Experience

**Thesis Mentor,** School of Materials Science and Engineering, Tongji University **Spring 2021/2020**
Mentored two undergraduates on their graduation theses.

- Provided topics and guide the design of calculation scheme.
- Taught calculation methods and software using.
- One was awarded with "outstanding graduates" title.

**Teaching Assistant,** School of Materials Science and Engineering, Tongji University **Fall 2020**
"Computational Materials Science" course for 87 undergraduate students.

- Helped solve technical problems in software installation and using.
- Exercise.

**Specialized Course Consultant,** Remedial Classes of Postgraduate Entrance Examination **Fall 2020/2019**
"Fundamentals of Materials Science" course for ~15 undergraduates who
want to apply for Master program in Materials Science at Tongji University.

## Publications

**Chen H**, Xiang H. P, First low-spin carbodiimide, $Fe_2(NCN)_3$, predicted from first-principles investigations. *Zeitschrift für Naturforschung B* 76(10-12): 783-788 (2021). https://doi.org/10.1515/znb-2021-0128

Ping D. H, **Chen H**, Xiang H. P, Formation of θ-$Fe_3C$ Cementite via θ′-$Fe_3C$ (ω-$Fe_3C$) in Fe–C Alloys. *Crystal Growth & Design* 21, 1683–1688 (2021). https://dx.doi.org/10.1021/acs.cgd.0c01533

Ping D. H, Xiang, H. P, **Chen H**, et al. A transition of ω-$Fe_3C$ → ω′-$Fe_3C$ →θ′-$Fe_3C$ in Fe-C martensite. *Scientific Reports* 10, 6081 (2020). https://doi.org/10.1038/s41598-020-63012-9

**Chen H**, Xiang H. P, Ping D. H, Stability of C atoms in γ-Fe, α-Fe, and ω-Fe in Fe-C alloys: A first-principles study. (In revision)

Contribute to:

Lu W. F, Wang Z. L, Xiang H. P, et al. Exploration of the atomic-level structures of the icosahedral clusters in Cu–Zr–Al ternary metallic glasses via first-principles theory. *Materials Research Express* 9, 065203 (2022) https://doi.org/10.1088/2053-1591/ac7516

## References


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