



# Chenxu Han

A 2nd-year PhD student of Xi'an Jiaotong University

Academic advisor: Professor Hongxiang Zong

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## EDUCATION

**Xi'an Jiaotong University | State Key Laboratory for Mechanical Behavior of Materials** 2021.09 - Now

Materials Science and Engineering | Academic PhD

Main Research Field: *Phase Transformation of Amorphous Materials*

**Xi'an Jiaotong University | State Key Laboratory for Mechanical Behavior of Materials** 2019.09-2021.07

Materials Science and Engineering | Academic Master

**GPA: 3.880 Ranking: 1/33**

Main Research Field: *Computational Materials Science and Materials Informatics*

**Chang'an University | School of Materials Science and Engineering** 2015.09-2019.07

Inorganic Non-metallic Materials | Bachelor Degree

**GPA: 2.820 Ranking: 14/60**

Undergraduate Thesis Topics: *Preparation and Performance Study About ZnO Fluorescent Quantum Dots*

## RESEARCH ARTICLES

[1] Sun S, Yang Y, Han C, et al. Unveiling the Grain Boundary-Related Effects on the Incipient Plasticity and Dislocation Behavior in Nanocrystalline CrCoNi Medium-Entropy Alloy. *Journal of Materials Science & Technology*, 2022, 127: 98-107.

◆ My contributions | The Molecular Dynamics Simulation Part: A spring-like dislocation motion was revealed under the grain boundary-related effects in nanocrystalline CrCoNi medium-entropy alloy, contrasting with the behavior in pure Ni.

[2] Liu X, Zheng L, Han C, et al. Identifying the Activity Origin of a Cobalt Single-Atom Catalyst for Hydrogen Evolution Using Supervised Learning. *Advanced Functional Materials*, 2021, 31(18): 2100547.

◆ My contributions | The Machine-Learning Part (refer to Fig. 4 in the article): A neural network model was built with the capability to accurately forecast the ratio of three distinct Co-occupied components based on experimentally obtained EXAFS curves.

[3] Yang Y, Zhao L, Han C, et al. Taking Materials Dynamics to New Extremes Using Machine Learning Interatomic Potentials. *Journal of Materials Informatics*, 2021, 1(2): 10.

◆ My contributions | Engage in the composition of articles and creation of artwork, with a specific focus on determining the content covering representations for local atomic environments in machine learning potentials.

[4] Han C, Yang Y, Luo Y, et al. GCNFF: A molecular dynamics force field developed by graph convolution neural network. *in work*.

◆ My contributions | The primary worker under the guidance of Professor Zong.

## ABOUT ME

**Skills:** 1. English ability: IELTS 6.5 (Listening 6.5, Speaking 6, Reading 7.5, Writing 6), College English Test Band 6 (CET-6);  
2. Certificate of Level 2 in National Computer Rank Examination (C programming language);  
3. Proficient utilization of Linux, Python, C++, MATLAB, Machine Learning and Neural Network algorithm;  
4. Computational materials science software: VASP, DPMD and LAMMPS.

**Specialties and Hobbies:** Roller skating, Table tennis, Jogging

**My strengths:**

1. Respects others, I'm willing to communicate with others and help them with a great sense of teamwork.
2. Serious, responsible and rigorous attitude towards work. Positive, optimistic attitude towards life.
3. With strong independent learning ability, I believe that diligence can compensate for incompetence.