High temperature superconductivity



ML predicttion of Tc

 $R^2 \approx 0.885$

 $low-T_c$

Fe-based

cuprates

Introduction

Superconductivity (SC) refers to the phenomenon where the electric resistivity of a material drops to zero at a certain temperature. The electrons are then promoted to a collected quantum state in which the electric current flow without dissipation. The Challenge was and still the realization of room temperature superconductivity (RTSC). 5 Nobel prices have been awarded to works related to SC.

1. Status of RTSC, records and trends

Hydrogen rich materials can achieve RTSC But requires extraordinary pressure. The challenge now is reducing the pressure rather then increasing the temperature

World record: 288 K at 260 GPa ⊆ ₁₅₀ ● HgBaCaCuO Run 1 HgBaCaCuO • Run 2 TiBaCaCuO Run 3 BiSrCaCuO FeSe films VBaCuO SmFeAsO BCS MgB₂ (La,Ba)₂CuO₄ Run 1 (p Run 2 (ρ) Outprates Nb₃Ge 🖲 LaOFeAs Run 3 (p) Bun 4 (p) Iron based Bun 1 (v Run 2 (7 250 P (GPa 100 200 300 400 Nature volume 586, pages373-377 (2020). Pressure (GPa) This article still under strong debate.

BCS Theory

Theory of Superconductivity J. Bardeen, L. N. Cooper, and J. R. Schrieffe Phys. Rev. 108, 1175 – Published 1 December 1957 Physics



BCS mechanis



2. New theoretical paradigms to understand and predict RTSC

140

100

80

60

20

20

40

80

measured T_c

npj Comput Mater 4, 29 (2018)

100 120 140

SC is a highly complicated many-body problem involing physics beyon the BOA and electron correlation beyond the LDA (PBE) xc functional. 120 Most recent theoretical developenmt are :



Phys. Rev. Lett. 125, 057001 (2020)

3. New approaches to design RTSC

Ab initio structure prediction accelerated with machine learning interatomic potentials (MLIP) using MAISE: Module for ab initio structure evolution (evolutionary algorithm)



Hajinazar S, et al. Comput. Phys. Commun. 259 107679 (2020).