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Biography

Dr. Shijun Zhao is an Assistant Professor at City University of Hong Kong. Dr. Zhao received his Bachelor's degree in Physics in 2008 and his Ph.D. degree in Nuclear Engineering in 2013, both from Peking University. His Ph.D. research centered on the radiation effects in ceramics and low-dimensional materials based on *ab initio* methods and molecular dynamics simulations. After graduation, Dr. Zhao conducted his postdoctoral research at the College of Engineering at Peking University for two years, with a focus on excited electron dynamics in materials under high-energy ion or laser irradiation using *ab initio* methods. Prior to joining City University of Hong Kong in 2018, he was a postdoctoral research associate at Oak Ridge National Laboratory, working on the irradiation effects in concentrated solid-solution alloys. Dr. Zhao's current research group works on Computational Defect Properties. Specifically, his group aims to understand defect thermodynamics, defect production, defect migration, and defect evolution in different materials under deformation or irradiation conditions. The defects considered include point defects, impurities, dislocations, stacking faults, grain boundaries, and surfaces, etc. The materials concerned including nuclear structural materials and nuclear fuels spanning from metallic alloys to ceramics. For this purpose, different simulation techniques at different scales are concurrently or sequentially employed. Dr. Zhao has authored and co-authored more than 50 technical papers with more than 1400 citations in the field of defect properties in materials.

Employment

Department of Mechanical Engineering
City University of Hong Kong
20 Aug 2018 → present

Research outputs

The stability of γ' precipitates in a multi-component FeCoNiCrTi_{0.2} alloy under elevated-temperature irradiation

Yeli, G., Chen, D., Yabuuchi, K., Kimura, A., Liu, S., Lin, W., Zhao, Y. & 2 others, Zhao, S. & Kai, J., Nov 2020, In : Journal of Nuclear Materials. 540, 152364.Scopus citations: 1

Defect evolution mechanism in U₃Si₂ from molecular dynamics simulations

Zhao, S., 15 Aug 2020, In : Journal of Nuclear Materials. 537, 152238.Scopus citations: 1

Effects of minor alloying addition on He bubble formation in the irradiated FeCoNiCr-based high-entropy alloys

Chen, D., Zhao, S., Sun, J., Tai, P., Sheng, Y., Yeli, G., Zhao, Y. & 4 others, Liu, S., Lin, W., Kai, W. & Kai, J., 14 Aug 2020, In : Journal of Nuclear Materials. 542, 152458.

Defect-Mediated Adsorption of Metal Ions for Constructing Ni Hydroxide/MoS₂ Heterostructures as High-Performance Water-Splitting Electrocatalysts

He, Z., Liu, Q., Zhu, Y., Tan, T., Cao, L., Zhao, S. & Chen, Y., 27 Jul 2020, In : ACS Applied Energy Materials. 3, 7, p. 7039-7047

Defect properties in a VTaCrW equiatomic high entropy alloy (HEA) with the body centered cubic (bcc) structure

Zhao, S., 1 May 2020, In : Journal of Materials Science and Technology. 44, p. 133-139Scopus citations: 2

On the role of heterogeneity in concentrated solid-solution alloys in enhancing their irradiation resistance

Zhao, S., 28 Apr 2020, In : Journal of Materials Research. 35, 8, p. 1103-1112Scopus citations: 4

高熵合金辐照性能的计算机模拟进展

徐彪, 付上朝, 赵仕俊 & 贺新福, 13 Apr 2020, In : 材料导报.

Fluctuations in stacking fault energies improve irradiation tolerance of concentrated solid-solution alloys

Zhao, S., Mar 2020, In : Journal of Nuclear Materials. 530, 151886.Scopus citations: 5

Alloying effects on low-energy recoil events in concentrated solid-solution alloys

Zhao, S., Liu, B., Samolyuk, G. D., Zhang, Y. & Weber, W. J., Feb 2020, In : Journal of Nuclear Materials. 529, 151941. Scopus citations: 2

Severe local lattice distortion in Zr- and/or Hf-containing refractory multi-principal element alloys

Tong, Y., Zhao, S., Bei, H., Egami, T., Zhang, Y. & Zhang, F., 15 Jan 2020, In : Acta Materialia. 183, p. 172-181Scopus citations: 10

Strain-tunable electronic properties and lithium storage of 2D transition metal carbide (MXene) Ti_2CO_2 as a flexible electrode

Li, Y., Li, N., Zhao, S., Fan, J. & Kai, J., 14 Jan 2020, In : Journal of Materials Chemistry A. 8, 2, p. 760-769Scopus citations: 4

Diffusion controlled helium bubble formation resistance of FeCoNiCr high-entropy alloy in the half-melting temperature regime

Chen, D., Zhao, S., Sun, J., Tai, P., Sheng, Y., Zhao, Y., Yeli, G. & 4 others, Lin, W., Liu, S., Kai, W. & Kai, J., 1 Dec 2019, In : Journal of Nuclear Materials. 526, 151747.Scopus citations: 7

Diffusion of point defects in ordered and disordered Ni-Fe alloys

Zhao, S., Osetsky, Y. & Zhang, Y., 15 Oct 2019, In : Journal of Alloys and Compounds. 805, p. 1175-1183Scopus citations : 6

Atomistic simulation of defect-dislocation interactions in concentrated solid-solution alloys

Zhao, S., Osetsky, Y. & Zhang, Y., Oct 2019, In : PHYSICAL REVIEW MATERIALS. 3, 10, 103602.Scopus citations: 2

Facile, cost-effective plasma synthesis of self-supportive FeS_x on Fe foam for efficient electrochemical reduction of N_2 under ambient conditions

Xiong, W., Guo, Z., Zhao, S., Wang, Q., Xu, Q. & Wang, X., 14 Sep 2019, In : Journal of Materials Chemistry A. 7, 34, p. 19977-19983Scopus citations: 10

Frenkel defect recombination in Ni and Ni-containing concentrated solid-solution alloys

Zhao, S., Osetsky, Y., Barashev, A. V. & Zhang, Y., Jul 2019, In : Acta Materialia. 173, p. 184-194Scopus citations: 10

Helium irradiated cavity formation and defect energetics in Ni-based binary single-phase concentrated solid solution alloys

Fan, Z., Zhao, S., Jin, K., Chen, D., Osetskiy, Y. N., Wang, Y., Bei, H. & 2 others, More, K. L. & Zhang, Y., 1 Feb 2019, In : Acta Materialia. 164, p. 283-292Scopus citations: 16

First-principles study of He behavior in a NiCoFeCr concentrated solid-solution alloy

Zhao, S., Chen, D. & Kai, J., 2019, In : Materials Research Letters. 7, 5, p. 188-193Scopus citations: 3

Local-environment dependence of stacking fault energies in concentrated solid-solution alloys

Zhao, S., Osetsky, Y., Stocks, G. M. & Zhang, Y., 2019, In : npj Computational Materials. 5, 13.Scopus citations: 25

A comparison study of local lattice distortion in $Ni_{80}Pd_{20}$ binary alloy and FeCoNiCrPd high-entropy alloy

Tong, Y., Zhao, S., Jin, K., Bei, H., Ko, J. Y. P., Zhang, Y. & Zhang, F. X., Nov 2018, In : Scripta Materialia. 156, p. 14-18 Scopus citations: 17

Irradiation responses and defect behavior of single-phase concentrated solid solution alloys

Yang, T., Li, C., Zinkle, S. J., Zhao, S., Bei, H. & Zhang, Y., 14 Oct 2018, In : Journal of Materials Research. 33, 19, p. 3077-3091Scopus citations: 15

Evolution of local lattice distortion under irradiation in medium- and high-entropy alloys

Tong, Y., Velisa, G., Zhao, S., Guo, W., Yang, T., Jin, K., Lu, C. & 6 others, Bei, H., Ko, J. Y. P., Pagan, D. C., Zhang, Y., Wang, L. & Zhang, F. X., Oct 2018, In : *Materialia*. 2, p. 73-81Scopus citations: 24

Local structure of NiPd solid solution alloys and its response to ion irradiation

Zhang, F. X., Ullah, M. W., Zhao, S., Jin, K., Tong, Y., Velisa, G., Xue, H. & 5 others, Bei, H., Huang, R., Park, C., Weber, W. J. & Zhang, Y., 30 Jul 2018, In : *Journal of Alloys and Compounds*. 755, p. 242-250Scopus citations: 3

Stability of vacancy-type defect clusters in Ni based on first-principles and molecular dynamics simulations

Zhao, S., Zhang, Y. & Weber, W. J., 1 Mar 2018, In : *Scripta Materialia*. 145, p. 71-75Scopus citations: 2

Effect of *d* electrons on defect properties in equiatomic NiCoCr and NiCoFeCr concentrated solid solution alloys

Zhao, S., Egami, T., Stocks, G. M. & Zhang, Y., Jan 2018, In : *PHYSICAL REVIEW MATERIALS*. 2, 1, 013602.Scopus citations: 44

Delayed damage accumulation by athermal suppression of defect production in concentrated solid solution alloys

Veliša, G., Wendler, E., Zhao, S., Jin, K., Bei, H., Weber, W. J. & Zhang, Y., 2018, In : *Materials Research Letters*. 6, 2, p. 136-141Scopus citations: 20

Ab Initio Study of Electronic Excitation Effects on SrTiO₃

Zhao, S., Zhang, Y. & Weber, W. J., 7 Dec 2017, In : *Journal of Physical Chemistry C*. 121, 48, p. 26622-26628Scopus citations: 1

Unique Challenges for Modeling Defect Dynamics in Concentrated Solid-Solution Alloys

ZHAO, S., WEBER, W. J. & ZHANG, Y., Nov 2017, In : *JOM*. 69, 11, p. 2084-2091Scopus citations: 23

Atomic-level heterogeneity and defect dynamics in concentrated solid-solution alloys

Zhang, Y., Zhao, S., Weber, W. J., Nordlund, K., Granberg, F. & Djurabekova, F., Oct 2017, In : *Current Opinion in Solid State and Materials Science*. 21, 5, p. 221-237Scopus citations: 76

Stacking fault energies of face-centered cubic concentrated solid solution alloys

Zhao, S., Stocks, G. M. & Zhang, Y., 1 Aug 2017, In : *Acta Materialia*. 134, p. 334-345Scopus citations: 107

Local Structure and Short-Range Order in a NiCoCr Solid Solution Alloy

Zhang, F. X., Zhao, S., Jin, K., Xue, H., Velisa, G., Bei, H., Huang, R. & 5 others, Ko, J. Y. P., Pagan, D. C., Neuefeind, J. C., Weber, W. J. & Zhang, Y., 19 May 2017, In : *Physical Review Letters*. 118, 20, 205501.Scopus citations: 92

X-ray absorption investigation of local structural disorder in Ni_{1-x}Fe_x (x = 0.10, 0.20, 0.35, and 0.50) alloys

Zhang, F. X., Jin, K., Zhao, S., Mu, S., Bei, H., Liu, J. C., Xue, H. Z. & 5 others, Popov, D., Park, C., Stocks, G. M., Weber, W. J. & Zhang, Y., 28 Apr 2017, In : *Journal of Applied Physics*. 121, 16, 165105.Scopus citations: 1

Additivity of kinetic and potential energy contributions in modification of graphene supported on SiO₂

Zhang, X., Zhao, S., Wang, Y. & Xue, J., 15 Apr 2017, In : *Nuclear Instruments and Methods in Physics Research, Section B: Beam Interactions with Materials and Atoms*. 397, p. 62-66

Atomic-scale dynamics of edge dislocations in Ni and concentrated solid solution NiFe alloys

Zhao, S., Osetsky, Y. N. & Zhang, Y., 15 Apr 2017, In : *Journal of Alloys and Compounds*. 701, p. 1003-1008Scopus citations: 24

Preferential diffusion in concentrated solid solution alloys: NiFe, NiCo and NiCoCr

Zhao, S., Osetsky, Y. & Zhang, Y., 15 Apr 2017, In : *Acta Materialia*. 128, p. 391-399Scopus citations: 55

Suppression of vacancy cluster growth in concentrated solid solution alloys

Zhao, S., Velisa, G., Xue, H., Bei, H., Weber, W. J. & Zhang, Y., 15 Feb 2017, In : Acta Materialia. 125, p. 231-237
Scopus citations: 29

Pressure-induced fcc to hcp phase transition in Ni-based high entropy solid solution alloys

Zhang, F. X., Zhao, S., Jin, K., Bei, H., Popov, D., Park, C., Neuefeind, J. C. & 2 others, Weber, W. J. & Zhang, Y., 2 Jan 2017, In : Applied Physics Letters. 110, 1, 011902.Scopus citations: 43

Defect energetics of concentrated solid-solution alloys from *ab initio* calculations: Ni_{0.5}Co_{0.5}, Ni_{0.5}Fe_{0.5}, Ni_{0.8}Fe_{0.2} and Ni_{0.8}Cr_{0.2}

Zhao, S., Stocks, G. M. & Zhang, Y., 14 Sep 2016, In : Physical Chemistry Chemical Physics. 18, 34, p. 24043-24056
Scopus citations: 60

Influence of chemical disorder on energy dissipation and defect evolution in advanced alloys

Zhang, Y., Jin, K., Xue, H., Lu, C., Olsen, R. J., Beland, L. K., Ullah, M. W. & 12 others, Zhao, S., Bei, H., Aidhy, D. S., Samolyuk, G. D., Wang, L., Caro, M., Caro, A., Stocks, G. M., Larson, B. C., Robertson, I. M., Correa, A. A. & Weber, W. J., 29 Aug 2016, In : Journal of Materials Research. 31, 16, p. 2363-2375Scopus citations: 56

Link between *K* absorption edges and thermodynamic properties of warm dense plasmas established by an improved first-principles method

Zhang, S., Zhao, S., Kang, W., Zhang, P. & He, X., 15 Mar 2016, In : Physical Review B. 93, 11, 115114.Scopus citations : 15

High adsorption capacity of heavy metals on two-dimensional MXenes: an *ab initio* study with molecular dynamics simulation

Guo, X., Zhang, X., Zhao, S., Huang, Q. & Xue, J., 7 Jan 2016, In : Physical Chemistry Chemical Physics. 18, 1, p. 228-233Scopus citations: 48

First-Principles Investigation to Ionization of Argon under Conditions Close to Typical Sonoluminescence Experiments

Kang, W., Zhao, S., Zhang, S., Zhang, P., Chen, Q. F. & He, X., 2016, In : Scientific Reports. 6, 20623.Scopus citations: 8

Modification of graphene supported on SiO₂ substrate with swift heavy ions from atomistic simulation point

Zhao, S. & Xue, J., Nov 2015, In : Carbon. 93, p. 169-179Scopus citations: 24

First-principles calculation of principal Hugoniot and K-shell X-ray absorption spectra for warm dense KCl

Zhao, S., Zhang, S., Kang, W., Li, Z., Zhang, P. & He, X., Jun 2015, In : Physics of Plasmas. 22, 6, 062707.

H⁺ (D⁺, T⁺)-beryllium collisions studied using time-dependent density functional theory

Zhao, S., Kang, W., Xue, J., Zhang, X. & Zhang, P., 6 Feb 2015, In : Physics Letters, Section A: General, Atomic and Solid State Physics. 379, 4, p. 319-326Scopus citations: 7

MXene nanoribbons

Zhao, S., Kang, W. & Xue, J., 28 Jan 2015, In : Journal of Materials Chemistry C. 3, 4, p. 879-888Scopus citations: 37

Comparison of electronic energy loss in graphene and BN sheet by means of time-dependent density functional theory

Zhao, S., Kang, W., Xue, J., Zhang, X. & Zhang, P., 21 Jan 2015, In : Journal of Physics Condensed Matter. 27, 2, 025401.Scopus citations: 16

Mechanism of the Defect Formation in Supported Graphene by Energetic Heavy Ion Irradiation: The Substrate Effect

Li, W., Wang, X., Zhang, X., Zhao, S., Duan, H. & Xue, J., 2015, In : Scientific Reports. 5, 9935.Scopus citations: 51

The potential application of phosphorene as an anode material in Li-ion batteries

Zhao, S., Kang, W. & Xue, J., 28 Nov 2014, In : Journal of Materials Chemistry A. 2, 44, p. 19046-19052Scopus citations: 195

Role of strain and concentration on the Li adsorption and diffusion properties on Ti_2C layer

Zhao, S., Kang, W. & Xue, J., 10 Jul 2014, In : Journal of Physical Chemistry C. 118, 27, p. 14983-14990 Scopus citations : 56

Manipulation of electronic and magnetic properties of M_2C (M = Hf, Nb, Sc, Ta, Ti, V, Zr) monolayer by applying mechanical strains

Zhao, S., Kang, W. & Xue, J., 31 Mar 2014, In : Applied Physics Letters. 104, 13, 133106. Scopus citations: 82

Gas adsorption on MoS_2 monolayer from first-principles calculations

Zhao, S., Xue, J. & Kang, W., 18 Mar 2014, In : Chemical Physics Letters. 595-596, p. 35-42 Scopus citations: 172

First-principles investigation of the intrinsic defects in Ti_3SiC_2

Zhao, S., Xue, J., Wang, Y. & Huang, Q., Mar 2014, In : Journal of Physics and Chemistry of Solids. 75, 3, p. 384-390 Scopus citations: 11

***Ab initio* study of irradiation tolerance for different $M_{n+1}AX_n$ phases: Ti_3SiC_2 and Ti_3AlC_2**

Zhao, S., Xue, J., Wang, Y. & Huang, Q., 14 Jan 2014, In : Journal of Applied Physics. 115, 2, 023503. Scopus citations: 62

Fabrication of nanopores in a graphene sheet with heavy ions: A molecular dynamics study

Li, W., Liang, L., Zhao, S., Zhang, S. & Xue, J., 21 Dec 2013, In : Journal of Applied Physics. 114, 23, 234304. Scopus citations: 44

Ion selection of charge-modified large nanopores in a graphene sheet

Zhao, S., Xue, J. & Kang, W., 21 Sep 2013, In : Journal of Chemical Physics. 139, 11, 114702. Scopus citations: 62

重离子辐照下石墨烯力学性能分子动力学研究

梁力, 赵仕俊, 王宇钢 & 薛建明, 20 May 2013, In : Beijing Daxue Xuebao (Ziran Kexue Ban)/Acta Scientiarum Naturalium Universitatis Pekinensis. 49, 3, p. 365-370 Scopus citations: 5

Mechanical properties of hybrid graphene and hexagonal boron nitride sheets as revealed by molecular dynamic simulations

Zhao, S. & Xue, J., 3 Apr 2013, In : Journal of Physics D: Applied Physics. 46, 13, 135303. Scopus citations: 85

Tuning the band gap of bilayer graphene by ion implantation: Insight from computational studies

Zhao, S. & Xue, J., Oct 2012, In : Physical Review B - Condensed Matter and Materials Physics. 86, 16, 165428. Scopus citations: 25

Influence of high pressure on the threshold displacement energies in silicon carbide: A Car-Parrinello molecular dynamics approach

Zhao, S., Xue, J., Lan, C., Sun, L., Wang, Y. & Yan, S., 1 Sep 2012, In : Nuclear Instruments and Methods in Physics Research, Section B: Beam Interactions with Materials and Atoms. 286, p. 119-123 Scopus citations: 6

Chemical bonding assisted damage production in single-walled carbon nanotubes induced by low-energy ions

Zhao, S., Xue, J., Wang, Y. & Yan, S., Aug 2012, In : Applied Physics A: Materials Science and Processing. 108, 2, p. 313-320 Scopus citations: 8

Effect of SiO_2 substrate on the irradiation-assisted manipulation of supported graphene: a molecular dynamics study

Zhao, S., Xue, J., Wang, Y. & Yan, S., 20 Jul 2012, In : Nanotechnology. 23, 28, 285703. Scopus citations: 35

Drilling nanopores in graphene with clusters: A molecular dynamics study

Zhao, S., Xue, J., Liang, L., Wang, Y. & Yan, S., 31 May 2012, In : Journal of Physical Chemistry C. 116, 21, p. 11776-11782 Scopus citations: 36

Self-irradiation of thin SiC nanowires with low-energy ions: A molecular dynamics study

Sun, L., Lan, C., Zhao, S., Xue, J. & Wang, Y., 4 Apr 2012, In : Journal of Physics D: Applied Physics. 45, 13, 135403.
Scopus citations: 5

Study on the effect of pressure on the properties of intrinsic point defects in monoclinic zirconia: *Ab initio* calculations

Zhao, S., Xue, J., Wang, Y. & Yan, S., 15 Feb 2012, In : Journal of Applied Physics. 111, 4, 043514. Scopus citations: 3

Grants

Projects

ECS: Effects of Doping Elements on the Irradiation Performance of Concentrated Solid-solution Alloys (High Entropy Alloys)

ZHAO, S.

1/10/19 → ...

MainGov: 多主元合金中辐照缺陷演化的决定性因素研究

ZHAO, S.

1/10/19 → ...