Influence of disorder on the electronic structure and electron-phonon coupling in the hexagonal high-entropy superconductor $(RuOs)_{0.7}(MoWZr)_{0.3}$

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Superconducting high-entropy alloys provide a unique platform for investigating the influence of chemical disorder on conventional phonon-mediated superconductivity. Although superconductivity in these materials is generally described within the Bardeen-Cooper-Schrieffer framework, the effects of disorder vary significantly from system to system, hindering the formulation of general conclusions regarding superconductivity in chemically disordered materials.

In this work, we investigate the hexagonal close-packed high-entropy superconductor $(RuOs)_{0.7}(MoWZr)_{0.3}$ [1] using first-principles calculations. The electronic structure is analysed using the coherent potential approximation within the Korringa-Kohn-Rostoker formalism (KKR-CPA) [2] and density functional theory supercell calculations performed with VASP [3,4]. Different approaches to modelling chemical disorder, including the virtual crystal approximation (VCA) and explicit disordered supercells, are systematically compared. Lattice dynamics and electron-phonon coupling are evaluated using VASP together with Phonopy [5], providing a comprehensive description of the superconducting properties.

The comparison of these computational approaches provides insight into the influence of structural and chemical disorder on the electronic structure, phonon spectra, electron-phonon coupling, and disorder-induced scattering of the electronic states. Particular attention is paid to the capabilities and limitations of the individual methods in describing highly disordered superconducting alloys. The presented results contribute to a deeper understanding of superconductivity in hexagonal high-entropy materials and provide guidance for future first-principles studies of chemically complex superconductors.

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References

[1] K Motla *et al.*, 2023 Supercond. Sci. Technol. 36 115024 (2023).
[2] S. Kaprzyk *et al.*, Phys. Rev. B 42, 7358 (1990).
[3] G. Kresse and J. Hafner, Phys. Rev. B 47, 558 (1993).
[4] G. Kresse and J. Furthmüller, Phys. Rev. B 54, 11169 (1996).
[5] A. Togo *et al.*, J. Phys.: Condens. Matter 35, 353001 (2023).