

First-principles investigation of structural, electronic, and magnetic properties of Fe-doped Cu₂O for spintronic applications

Ibrahim Ismail Idowu^{1*}, Nuhu Yunusa² and Margaret Adebimpe Umeche³

¹Department of Physics, Federal University Dutse, Dutse 720101, Nigeria.

²Department of Physics, Baze University, Abuja, Nigeria.

³Department of Physics, Kogi State University, Kabba, Nigeria.

*Corresponding author. Email: dridowuaraba@gmail.com

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ABSTRACT: This study employs spin-polarised density functional theory (GGA PBE+U) to investigate the structural, electronic, and magnetic properties of Fe-substituted Cu₂O at a nominal dopant concentration of 2.08%, corresponding to one Fe atom in a 2×2×2 supercell (48 atoms). The optimised lattice constant of pristine Cu₂O (4.252 Å) agrees closely with the experimental JCPDS value (4.2696 Å), with a relative error of only 0.4%. Upon Fe substitution, the lattice constant decreases to 4.018 Å, and the Fe–O bond length (1.804 Å) becomes shorter than the original Cu–O bond (1.841 Å), indicating local lattice contraction. The negative formation energy (−7.67 eV) confirms that Fe incorporation is thermodynamically favourable under Cu-poor growth conditions. While a local bond angle change from 109.47° to 104.80° is observed, the overall cubic symmetry of Cu₂O is preserved. Pristine Cu₂O shows symmetric spin channels with a semiconducting gap and no net spin polarisation. In contrast, Fe substitution introduces Fe 3d-derived impurity states near the Fermi level, leading to strong spin asymmetry: one spin channel becomes metallic while the other remains semiconducting, resulting in near-half-metallic behaviour. Projected density of states reveals strong hybridisation between Fe 3d and O 2p orbitals, which underlies the observed exchange splitting and spin polarisation. The computed total magnetic moment is approximately 3.05 μB per Fe atom, largely localised on the Fe site with minor polarisation on neighbouring O and Cu atoms, which is a hallmark of dilute magnetic semiconductors. Comparison of ferromagnetic (FM) and antiferromagnetic (AFM) configurations shows that the FM state is lower in energy by 0.24 eV, establishing an FM ground state. Using the mean-field approximation, the Curie temperature is estimated to be about 185 K, suggesting that room-temperature ferromagnetism may be achievable with higher doping concentrations or co-doping strategies. These results highlight Fe-doped Cu₂O as a promising candidate for spintronic applications.

Keywords: Cuprous oxide, density functional theory, dilute magnetic semiconductor, Fe doping, half-metallicity, spintronics.

INTRODUCTION

Oxide semiconductors have maintained their position at the forefront of materials research due to their exceptional chemical robustness, natural abundance, and versatile applicability across energy conversion and environmental

remediation technologies (Danish *et al.*, 2020; Masroor, 2022). Among this material family, cuprous oxide (Cu₂O) distinguishes itself through several compelling attributes. These include a direct band gap positioned within the

visible spectrum, intrinsic p-type conductivity that eliminates the need for extrinsic doping in many applications, environmental compatibility, and remarkably low production costs (Marathey *et al.*, 2022; Baran *et al.*, 2021). These characteristics have propelled Cu₂O into the spotlight for diverse applications, including photocatalytic water splitting, solar energy harvesting, gas sensing technologies, and various optoelectronic devices (Su *et al.*, 2023; Abdullahi *et al.*, 2025).

The crystallographic architecture of Cu₂O features a cubic lattice wherein Cu⁺ ions establish linear coordination with oxygen atoms. This distinctive structural arrangement gives rise to a closed-shell 3d¹⁰ electronic configuration (all d-orbitals are fully occupied with paired electrons), fundamentally explaining the absence of intrinsic magnetic ordering in pristine Cu₂O (Bogenrieder *et al.*, 2024). In its common oxidation state in Cu₂O, copper exists as Cu⁺ (cuprous ion) with the configuration: 1s² 2s² 2p⁶ 3s² 3p⁶ 3d¹⁰.

The valence band architecture derives predominantly from hybridised Cu 3d and O 2p states, while the conduction band is primarily constituted by Cu 4s states. Although this electronic configuration facilitates efficient optical absorption and charge carrier transport, the absence of magnetic ordering presents a significant barrier to integration with spin-based electronic architectures.

Recent advances in defect engineering and substitutional doping have demonstrated remarkable potential for tailoring the physical properties of Cu₂O (Fadlallah *et al.*, 2016; Živković *et al.*, 2019; Okoye *et al.*, 2023). Transition metal incorporation, in particular, has emerged as a powerful strategy for manipulating both electronic and magnetic behaviour. Iron (Fe) presents an especially attractive dopant candidate, as its partially filled 3d orbitals can generate localised magnetic moments and mediate exchange interactions within the host lattice (Abdelfatah *et al.*, 2022). The strategic importance of such doping approaches is underscored by growing interest in dilute magnetic semiconductors for spintronic applications (Zhao *et al.*, 2019; Gupta *et al.*, 2020).

Contemporary experimental and theoretical investigations have established that Fe incorporation substantially modifies the electronic structure of Cu₂O, with the potential to induce magnetic ordering (Li *et al.*, 2015; Satheeskumar *et al.*, 2018). However, the resulting properties exhibit strong sensitivity to dopant concentration, oxidation state, and local atomic coordination environment. This complexity necessitates systematic first-principles investigation to elucidate the microscopic origins of magnetism in Fe-doped Cu₂O systems. Fe (1s²2s²2p⁶3s²3p⁶3d⁶4s²) is selected due to its partially filled 3d orbitals (3d⁶ 4s²), high magnetic moment, and excellent solubility in oxide hosts. The 2.08% concentration corresponds to one Fe substitution in a 2×2×2 supercell (Figure 1), balancing computational cost with experimental relevance. Higher concentrations (2%,

4.17%, 8.33%) are planned for future work to determine maximum Iron (Fe) incorporation limits.

The novelty of this work lies in the systematic atomistic characterisation of Fe-induced magnetism in Cu₂O, including quantification of exchange splitting, impurity band formation, and spin density localisation. This study, therefore, systematically investigates Fe substitution in Cu₂O using spin-polarised DFT to clarify structural feasibility, electronic reconstruction, and magnetic origin, providing a theoretical foundation for developing Cu₂O-based spintronic devices such as spin valves and magnetic tunnel junctions.

METHODOLOGY

All calculations were performed within the spin-polarised density functional theory (DFT) framework as implemented in the Quantum ESPRESSO package (Giannozzi *et al.*, 2017). The Kohn–Sham equations

$$\left[-\frac{\hbar^2}{2m_e} \nabla^2 + V_{\text{eff}}(\mathbf{r}) \right] \psi_i(\mathbf{r}) = \varepsilon_i \psi_i(\mathbf{r}),$$

The Kohn–Sham equations were solved self-consistently, with the effective potential given by $V_{\text{eff}}(\mathbf{r}) = V_{\text{ext}}(\mathbf{r}) + V_{\text{H}}(\mathbf{r}) + V_{\text{xc}}(\mathbf{r})$, where $V_{\text{ext}}(\mathbf{r})$ is the external ionic potential, $V_{\text{H}}(\mathbf{r})$ is the Hartree potential, and $V_{\text{xc}}(\mathbf{r})$ is the exchange–correlation potential.

The exchange–correlation interaction was described using the generalized gradient approximation (GGA) in the Perdew–Burke–Ernzerhof (PBE) parameterisation. Ultrasoft pseudopotentials were employed to represent electron–ion interactions, following established practices for transition metal oxide systems (Hafner, 2008).

Due to computational constraints, HSE06 calculations were not performed in this study. Instead, we employed DFT+U within the GGA-PBE framework, applying a Hubbard U correction of 8.5 eV to the Cu d electrons to better describe the localised electronic states. We acknowledge that GGA-PBE typically underestimates band gaps, and the addition of DFT+U improves the description of strong electron correlation but does not fully remedy the band-gap problem. Future work will employ the HSE06 hybrid functional to obtain more accurate band gaps. Nonetheless, our GGA-PBE+U results remain valid for comparative analysis of doping-induced changes.

Through systematic convergence testing, a plane-wave kinetic energy cutoff of 45 Ry and a charge density cutoff of 350 Ry were selected to ensure reliable total energies and accurate structural optimisation. Brillouin zone integrations were performed using a 4 × 4 × 4 Monkhorst–Pack k-point mesh for self-consistent calculations, providing adequate sampling for the supercell geometry.

To simulate Fe doping, a 2 × 2 × 2 supercell of cubic Cu₂O was constructed containing 48 atoms. One Cu

atom was substituted with Fe, yielding a dopant concentration of 2.08%. This value is well within the dilute doping regime that minimises artificial dopant–dopant interactions while remaining experimentally accessible (Nolan *et al.*, 2008). Structural relaxation was performed until atomic forces fell below 10^{-3} Ry/Bohr and total energy converged to within 10^{-6} Ry. Spin polarisation was explicitly incorporated throughout all calculations to capture magnetic effects accurately. For detailed electronic structure analysis, non-self-consistent calculations were performed using the tetrahedron method, and spin-resolved band structures alongside density of states (DOS) were systematically analysed. To identify whether the system favours ferromagnetic (FM) or antiferromagnetic (AFM) ordering, we perform spin-polarized DFT calculations on a supercell containing multiple magnetic atoms.

RESULTS AND DISCUSSION

Structural stability and thermodynamic feasibility

The defect formation energy for substitutional Fe at the Cu site is given by the standard expression:

$$E_f = E_{\text{Fe:Cu}_2\text{O}} - E_{\text{Cu}_2\text{O}} - \mu_{\text{Fe}} + \mu_{\text{Cu}}$$

where: $E_{\text{Fe:Cu}_2\text{O}}$ and $E_{\text{Cu}_2\text{O}}$ are the total energies of the Fe-doped and pristine 48-atom supercells, respectively (Figure 1) and μ_{Fe} and μ_{Cu} are the chemical potentials of Fe and Cu.

All chemical potentials are referenced to their respective standard states (bulk metals or O₂ molecule). The reported formation energy of -7.67 eV corresponds to the Cu-poor / Fe-rich condition, which thermodynamically favors substitution of Fe onto the Cu site. Under Cu-rich conditions, the formation energy becomes less negative (or positive), confirming that Cu-poor growth environments are necessary for stable Fe incorporation.

The computed formation energy for Fe substitution at the Cu site is negative under appropriate chemical conditions, confirming thermodynamic feasibility. Energetically favourable substitution of transition metals into Cu₂O has been reported in both theoretical and experimental investigations, particularly under Cu-poor growth environments (Jamal *et al.*, 2021).

The optimised lattice constant of pristine Cu₂O (4.252 Å) agrees closely with the experimental JCPDS reference value of 4.2696 Å (JCPDS 05-0667), corresponding to a relative error of only 0.4%. Upon 2.08% Fe substitution, our calculated lattice constant decreases to 4.018 Å, a contraction that is consistent with the experimental observations of Abdelfatah *et al.* (2022) for Fe-doped Cu₂O thin films. Alongside this lattice reduction, the metal–

oxygen bond length shortens from 1.841 Å (Cu–O) to 1.804 Å (Fe–O) (Table 1). These trends are in line with prior first-principles studies on transition-metal doping and defect-induced lattice relaxation in Cu₂O.

Hybrid DFT calculations reported by Zivković *et al.* (2019) indicate that substitutional transition-metal dopants in Cu₂O promote pronounced local structural relaxation accompanied by enhanced metal–oxygen hybridisation. This increased hybridisation strengthens the TM–O interaction, resulting in shorter bond lengths and an overall lattice contraction. In a similar context, defect investigations by Scanlon *et al.* (2009) highlighted the importance of local bonding distortions and strong Cu–O hybridisation in stabilising defect states within Cu₂O, further demonstrating that substitutional incorporation or defect-related perturbations intrinsically lead to localised lattice contraction.

Although a local distortion is observed, reflected by the bond angle change from 109.47° to 104.80°, the overall cubic symmetry of Cu₂O is preserved. This indicates that the structural modification is confined to the dopant's local environment without altering the global phase. This finding is consistent with experimental XRD studies of Fe-doped Cu₂O thin films. Abdelfatah *et al.* (2022) reported retention of the characteristic cubic Cu₂O diffraction pattern at low Fe concentrations, with no detectable secondary phases. Only slight peak shifts were observed, suggesting subtle lattice variation due to substitutional incorporation rather than phase segregation. Thus, the present results support intrinsic substitutional Fe incorporation while maintaining the cubic Cu₂O structure.

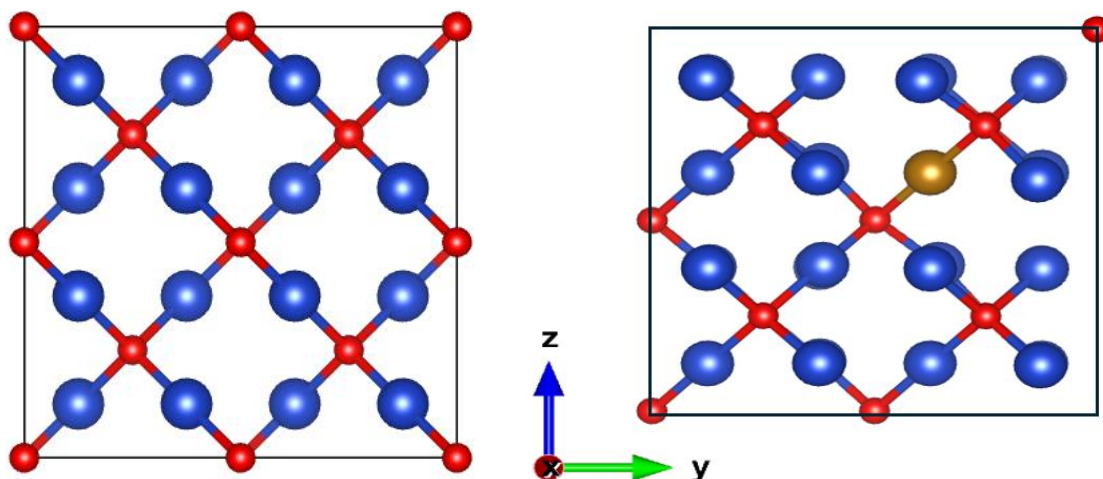
Electronic structure reconstruction

Spin-resolved band structure

Pristine Cu₂O exhibits zero magnetic moment due to the closed-shell electronic configuration of Cu⁺ (3d¹⁰), in which all d-orbitals are fully occupied, and spin-up and spin-down states are completely balanced, resulting in diamagnetic behaviour (Bogenrieder *et al.*, 2024). Upon substitution of Cu with Fe, a finite total magnetic moment of approximately 3.05 μB emerges, indicating the introduction of unpaired 3d electrons from the Fe dopant. This value suggests partial occupancy of Fe-3d orbitals consistent with Fe²⁺ (3d⁶) or Fe³⁺ (3d⁵) states under crystal field splitting within the Cu₂O lattice. The magnetic moment is predominantly localised on the Fe atom (Liyanaage *et al.*, 2020), while neighbouring Cu and O atoms exhibit negligible spin polarisation, demonstrating that the magnetism is dopant-centred rather than host-mediated. The asymmetry between spin-up and spin-down bands observed in Fig. 3 directly explains the origin of this magnetic behavior, as the unequal distribution of occupied electronic states in the two spin channels produces a net

Table 1. Structural parameters and formation energy of pristine and Fe-doped Cu_2O .

Parameter	Pristine Cu_2O	Fe-doped Cu_2O
Lattice constant (Å)	4.2520	4.0180
Cu–O / Fe–O (Å)	1.8412	1.8044
Cu–Cu / Fe–Cu (Å)	3.0066	2.9087
Bond angle (°)	109.471	104.796
Formation energy (eV)	—	-7.66952

**Figure 1.** Optimized crystal structures of (a) pristine Cu_2O and (b) Fe-substituted Cu_2O (2.08% Fe concentration). The Fe, Copper and Oxygen atom are highlighted in Brown, blue, and red colour.

spin imbalance according to $M = N_{\uparrow} - N_{\downarrow}$. This exchange splitting of Fe-3d states near the Fermi level leads to spin polarization without destroying the overall semiconducting nature of the system. The spin density isosurface further confirms that the magnetic moment is strongly localised around the Fe dopant, with only minimal induced polarisation on surrounding atoms, indicating short-range magnetic interaction and dilute character. The coexistence of a preserved band gap and a finite localised magnetic moment therefore establishes Fe-doped Cu_2O as a dilute magnetic semiconductor, in which semiconducting transport and dopant-induced magnetism are simultaneously maintained, making the material potentially relevant for spintronic and magneto-optoelectronic applications.

Density of states and orbital hybridisation

The total density of states (DOS) (Figure 2) reveals clear spin polarisation, with a non-zero DOS at the Fermi level in one spin channel and a reduced density in the opposite channel, indicating the formation of spin-split impurity states upon Fe substitution.

Projected DOS analysis (Figure 3) shows that states near the Fermi level are dominated by Fe 3d orbitals, which strongly hybridise with O 2p states. This dopant–host orbital interaction underlies the observed exchange splitting and spin asymmetry. Such hybridisation-driven impurity states are widely recognised as a key mechanism for dopant-induced magnetism in oxide semiconductors, where the overlap of transition-metal 3d and oxygen 2p orbitals generates spin-polarised states that mediate magnetic coupling (Mahmood *et al.*, 2023).

In pristine Cu_2O , Cu 3d states are predominantly located deep within the valence band, confirming that the electronic reconstruction observed upon Fe substitution is driven by the dopant rather than intrinsic host band structure modifications. The emergence of Fe-induced mid-gap states provides a plausible explanation for the experimentally observed optical band-gap narrowing in Fe-doped cuprous oxide systems. For instance, optical absorption measurements on Fe-doped $\text{Cu}_2\text{O}/\text{CuO}$ heterostructures report a reduced effective band gap compared to undoped Cu_2O , attributed to Fe-related impurity levels that enable sub-bandgap transitions under visible illumination. These findings are consistent with mid-gap state formation and enhanced carrier generation near

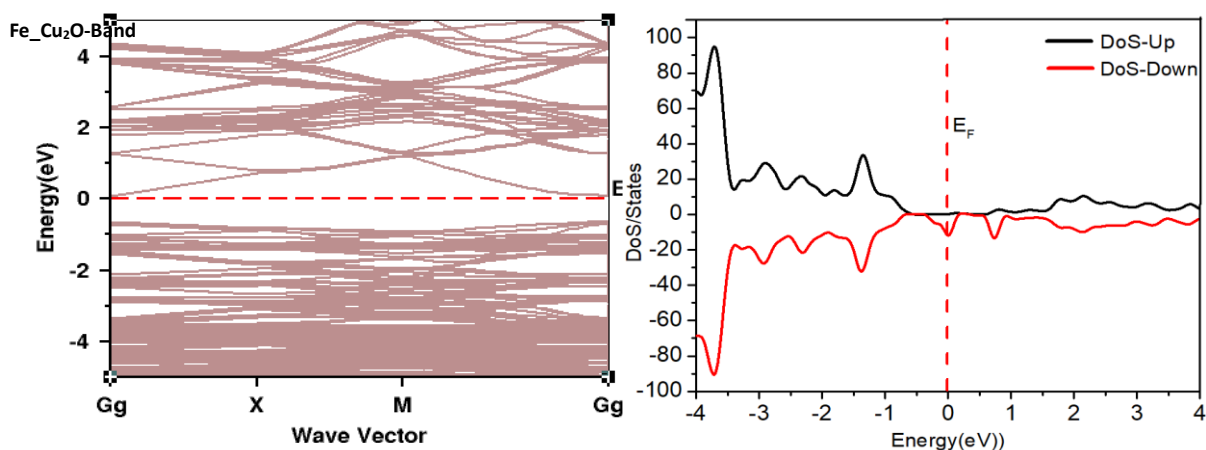


Figure 2. Spin-polarized electronic band structure (left) and total density of states (right) of Fe-doped Cu_2O , showing pronounced spin asymmetry. The red dashed line indicates the Fermi level position.

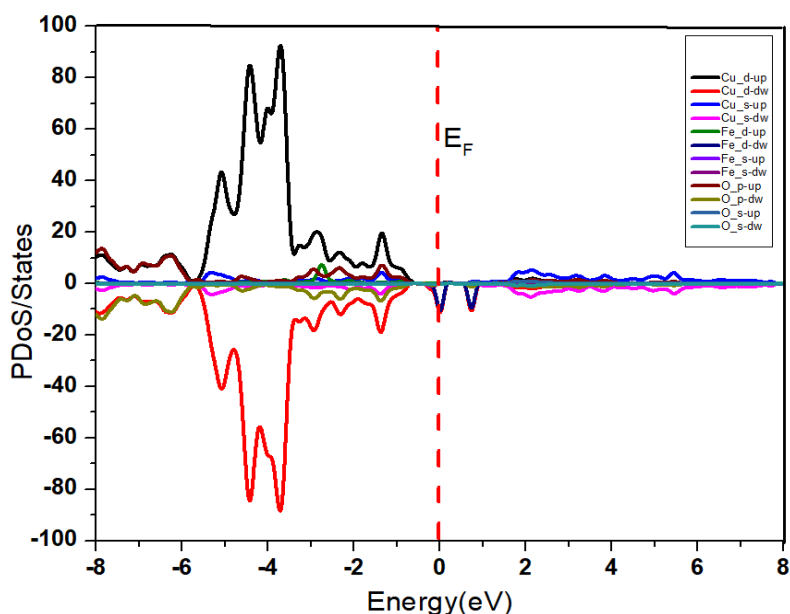


Figure 3. Projected density of state showing impurities along the spin-down orbit.

the band edges (Uma *et al.*, 2022). Collectively, these results indicate that Fe substitution introduces localised states within the Cu_2O band gap, leading to a narrowed optical gap and modified electronic transitions absent in the pristine material.

Magnetic properties and spin localization

Pristine Cu_2O is diamagnetic, exhibiting zero net magnetic moment due to its filled $3d^{10}$ configuration, as confirmed by spin-polarised first-principles calculations showing

negligible magnetisation in the ideal bulk structure (Bogenrieder *et al.*, 2024).

Upon low-concentration Fe substitution, first-principles studies predict a local magnetic moment of approximately $3 \mu\text{B}$ per Fe atom, reflecting the high-spin configuration of Fe arising from its partially filled 3d orbitals and crystal field environment. For instance, density functional theory investigations of oxide superlattices containing FeO indicate that the high-spin state is energetically favoured, producing significant local moments that capture the intrinsic magnetic character of Fe in oxide hosts (Gao *et al.*, 2024).

Spin-density visualisations in doped systems (Figure 4) reveal strong magnetisation localised around the Fe site, with minimal polarisation induced on neighbouring host cations, a hallmark of dopant-centred magnetism in dilute magnetic semiconductors (DMSs). This behaviour originates from the localised exchange splitting of Fe 3d states, which lifts spin degeneracy and establishes robust magnetic polarisation while preserving the semiconducting nature of the host.

The total energies of ferromagnetic (FM) and antiferromagnetic (AFM) spin configurations were compared. The energy difference is defined as:

$$\Delta E = E_{\text{AFM}} - E_{\text{FM}}$$

Here, the FM configuration is lower in energy by $\Delta E = 0.24$ eV, indicating an FM ground state. Using the mean-field approximation, the Curie temperature is estimated via:

$$T_c = \frac{2\Delta E}{3k_B}$$

Where k_B is Boltzmann's constant (8.617×10^{-5} eV/K). Substituting $\Delta E = 0.24$ eV gives $T_c \approx 185$ K. This suggests that while the pristine system is below room temperature, potential for room-temperature applications may be achieved with higher doping.

Experimental studies on Fe-doped magnetic oxides have reported ferromagnetic behaviour at room temperature, and first-principles calculations confirm that substitutional Fe incorporation alone is sufficient to generate localised moments without the need for secondary phases (Li *et al.*, 2024).

Fe spin state analysis

Spin-polarised DFT results show that magnetism in Fe-doped Cu_2O is dominated by the Fe dopant, with minor induced moments on neighbouring O atoms due to p-d hybridization, while Cu atoms remain nearly non-magnetic. The Fe atom exhibits a large local magnetic moment ($\sim 3\text{--}4$ μB), indicating a high-spin configuration arising from partially filled Fe 3d states and exchange splitting (the energy difference between spin-up and spin-down states due to electron-electron interactions) near the Fermi level.

Upon substitution into the Cu^+ site, iron is expected to adopt an oxidation state of Fe^{2+} ($3d^6$) or Fe^{3+} ($3d^5$). The high-spin configuration (Fe^{2+} with $t_{2g}^4 e_g^2$) yields a local magnetic moment consistent with the computed value of ~ 3 μB . The spin density is strongly localised around Fe with slight delocalisation onto adjacent O atoms, implying impurity-driven magnetism mediated by superexchange interactions. Therefore, Fe incorporation induces stable

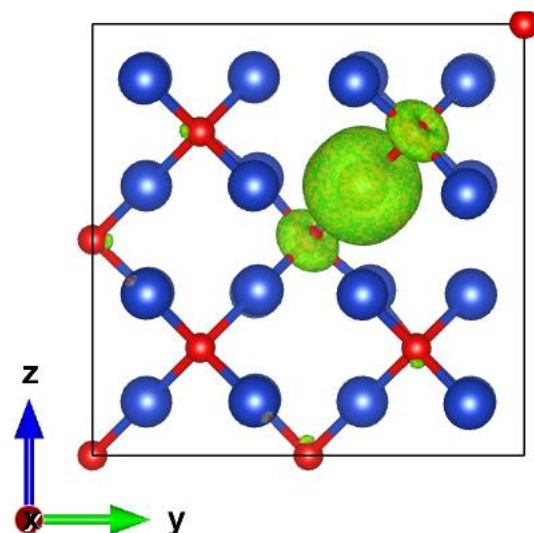


Figure 4. Spin density isosurface of Fe-doped Cu_2O illustrating localized magnetism around the Fe dopant site.

local magnetic moments without disrupting the Cu_2O lattice, highlighting its suitability for spintronic applications.

Conclusion

This study employed spin-polarized density functional theory (GGA-PBE+U) to investigate Fe-substituted Cu_2O at a nominal dopant concentration of 2.08%, which corresponds to one Fe atom in a $2 \times 2 \times 2$ supercell containing 48 atoms. The optimised lattice constant of pristine Cu_2O (4.252 Å) agrees closely with the experimental JCPDS value (4.2696 Å), with a relative error of only 0.4%. Upon Fe substitution, the lattice constant decreases to 4.018 Å, and the Fe–O bond length (1.804 Å) becomes shorter than the original Cu–O bond (1.841 Å), indicating local lattice contraction. The formation energy of Fe substitution at the Cu site is negative (-7.67 eV), confirming that Fe incorporation is thermodynamically favourable under Cu-poor growth conditions. Although a local bond-angle change from 109.47° to 104.80° is observed, the overall cubic symmetry of Cu_2O is preserved, consistent with experimental XRD observations. Pristine Cu_2O exhibits symmetric spin channels with a clear semiconducting gap and no net spin polarisation. Fe substitution introduces Fe-3d derived impurity states near the Fermi level, leading to pronounced spin asymmetry. One spin channel becomes metallic while the other remains semiconducting, resulting in near half-metallic behavior that is highly desirable for spintronic applications. Projected density of states reveals strong hybridisation between Fe-3d and O-2p orbitals, which is the microscopic origin of the observed exchange splitting

and spin polarisation. The computed total magnetic moment is approximately 3.05 μ_B per Fe atom, largely localised on the Fe site with only minor polarisation on neighbouring O and Cu atoms, a hallmark of dilute magnetic semiconductors. Comparison of ferromagnetic (FM) and antiferromagnetic (AFM) configurations shows that the FM state is lower in energy by 0.24 eV, establishing an FM ground state. Using the mean-field approximation, the Curie temperature is estimated to be about 185 K, suggesting that room-temperature ferromagnetism may be achievable with higher doping concentrations or co-doping strategies.

Recommendation

Limitations of this study include band-gap underestimation by GGA-PBE+U, the need to explore a wider range of dopant concentrations (e.g., 2%, 4.17%, 8.33%), and the absence of elastic constant and phonon calculations. Future work should employ the HSE06 hybrid functional for more accurate electronic structures and perform experimental validation (XMCD, SQUID magnetometry, ESR) to confirm the predicted magnetic properties. Overall, this study demonstrates that Fe doping is a viable route to convert non-magnetic Cu₂O into a dilute magnetic semiconductor, providing a theoretical foundation for developing Cu₂O-based spintronic devices such as spin valves, magnetic tunnel junctions, and spin-light emitting diodes.

CONFLICT OF INTEREST

The authors declare that they have no conflict of interest.

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