Unraveling Hydrogen Defects in Delafossite $CuMO_2$: Impact on p-Type Conductivity and Vibrational Signatures

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Transparent conducting oxides with p-type conductivity hold immense potential for various optoelectronic applications. Among them, delafossite $CuMO_2$ (M = Al, Ga, In) has been widely studied, with its *p*-type conductivity attributed to native acceptor defects, particularly copper vacancies (V_{Cu}). However, the interplay between these defects and hydrogen impurities remains a critical factor affecting the electrical properties of these materials. Using range-separated hybrid density functional calculations, we investigate the influence of hydrogen on defect passivation, electronic conductivity, and local vibrational properties.

Our findings reveal that hydrogen form stable defect complexes, such as H_i-V_{Cu} and $2H_i$-V_{Cu}, effectively passivating copper vacancies and reducing hole concentration. The formation of H_i-Cu_M complexes is also expected, though with lower binding energies, suggesting their potential dissociation at moderate temperatures. These interactions indicate that hydrogen incorporation plays a pivotal role in governing *p*-type conductivity of $CuMO_2$ under different synthesis conditions.[1]

In addition to electronic effects, predictions of local vibrational modes (LVMs) associated with hydrogen-related defects in $CuMO_2$ are also presented, with calculated frequencies ranging from ~2,800 cm^{-1} to ~3,800 cm^{-1}. These distinct vibrational signatures, particularly for H_i, H_i-V_{Cu}, and $2H_i$-V_{Cu} defects, offer a valuable reference for experimental investigations using infrared (IR) spectroscopy. Identifying IR-active modes of these hydrogen-related defects provides a pathway for detecting hydrogen incorporation and defect interactions in delafossite oxides.

References

1. Ananchuensook, A.; Chatratin, I.; Janotti, A.; Watcharatharapong, T.; T-Thienprasert, J; Boonchun, A.; Jungthawan, S.; Reunchan, P. Journal of Applied Physics, **2024**, 135, 185705.

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