From moisture sensitivity of CuI to new research directions for p-type transparent conductors

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In the first part of this talk, I will discuss the unexpected behavior we found in gas-phase iodized CuI when exposed to different humidity levels [1]. Even though many metal iodides are hygroscopic, the effect of moisture on the electrical properties of CuI had not yet been clarified We observed a 2-fold increase in the conductivity of fresh CuI after exposure to ambient humidity for 5 h, followed by slight long-term degradation. Simultaneously, the work function of CuI decreased by almost 1 eV, which could explain the large spread in previously reported work function values. The conductivity increase is partially reversible and is maximized at intermediate humidity levels. On the basis of the large intragrain mobility measured by THz spectroscopy, we suggest that hydration of grain boundaries may be beneficial for the overall hole mobility.

In the second part of this talk, I will discuss our experimental implementation of a recently proposed design criterion for p-type transparent conductors. The criterion is choosing materials with (i) a relatively narrow - but indirect - band gap, and (ii) a large energy difference between the indirect band gap and the first available direct transitions [1,2]. Low band gap materials have the advantage of often having low hole effective masses and shallow valence bands, usually enabling high-hole mobilities and concentrations. The large energy difference between the indirect and direct band gaps could ensure good transparency as long as the material is not too thick (as in thin film samples).

Using a unique combinatorial sputter chamber with reactive PH_3 gas, we synthesized two thin-film materials expected to satisfy these requirements: BP and CaCuP. We found that the hole conductivity of CaCuP under optimized growth conditions was almost on par with the conductivity of state-of-the-art n-type TCMs even in the absence of any extrinsic dopant. Indirect absorption was stronger than expected, but we believe that improved crystal quality might mitigate it by an order of magnitude. The field of metal phosphides appears to be a fertile search space for potential p-type transparent conductors and optoelectronic materials in general.

[1] Crovetto *et al.,* ACS Appl. Mater. Interfaces, **12,** 48741–48747 (2020)
[2] B. Williamson *et al.,* Chem. Mater., **29,** 2402–2413 (2017)
[3] J. Varley *et al.,* Chem. Mater., **29,** 2568–2573 (2017)