Exploring the Sb (V) oxides: transport and defect properties of ASb_2O_6 (A = Mg, Ca, Sr, Ba, Cd)

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Transparent conducting oxides (TCOs) possess a unique combination of optical transparency and electrical conductivity, making them essential for numerous optoelectronic applications including electron transport layers in solar cells [1-3]. However, the number of oxides that are both transparent to visible light and exhibit the metallic-like conductivity required for such applications is limited to a few well-established systems. Recently, $ZnSb_2O_6$ and Sb_2O_5 have been proposed as promising Sb(V)-based oxides [4,5,6], demonstrating transparent conducting behavior, unusually deep band edges, and interesting band alignment for optoelectronic applications. Building on the promising results of these two systems, we extended our exploration to ASb_2O_6 compounds (A = Mg, Ca, Sr, Ba, Cd) in search of alternative candidates for practical TCO applications. Our findings indicate that $CdSb_2O_6$ and $MgSb_2O_6$ exhibit excellent transport and optical properties, positioning them as strong contenders for the future of TCOs. The defect chemistry of these two oxides was also investigated, providing valuable insights into their behavior for working applications. Finally, our work reveals a strong correlation between the atomic packing factor (a measure of how efficiently atoms are packed in a crystal structure) and carrier mobility, offering a potential approach for rapid screening of promising candidates within this class of materials.

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