

## Understanding and optimizing the electronic properties of CuI p-type transparent semiconductors

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Copper iodide in the zincblende phase is a naturally p-type transparent semiconductor with record hole conductivity. A key step to enable applications of this promising material, e.g., for transparent electronics is the possibility to control and optimize its electronic properties. In this presentation I will discuss the effects of defects [1,2], doping [2] and alloying [3], as well as the properties of different CuI phases [4] and stoichiometries [1].

Our work relies on first-principles density functional theory and accurate thermodynamic analysis, as well as on the development of efficient high-throughput computational workflows. I will show that the calculations performed up to now lead already to a better understanding of CuI materials properties and provide specific suggestions on how to enhance p-type conductivity by doping and alloying.

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- [2] M. Graužinyte, S. Botti, M.A.L. Marques, S. Goedecker, and J.A. Flores-Livas, *Phys. Chem. Chem. Phys.* **21**, 18839–18849 (2019) – inside front cover, selected as a 2019 HOT PCCP Article
- [3] M. Seifert, M.A.L. Marques, and S. Botti, in preparation
- [4] M. Seifert, M. Kawashima, C. Rödl, and S. Botti, *J. Mater. Chem. C* **9**, 11284–11291 (2021)