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Tailor-Making Chalcopyrite Alloys for 100-Nm Thin Solar Cells

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Emerging Cu-based materials are explored to benefit from the energetically high-lying Cu d-state in combination with low effective mass of the minority carriers. Materials with higher functionality open for ultrathin devices and thereby less raw material usage. In this talk, we discuss the details in the optoelectronic properties of emerging Cu-based chalcopyrites, like for instance Cu2(Sn,Ge)S3, Cu3Sb(S,Se)3, Cu3Bi(S,Se)3, and Cu2XSnS4 (X = transition metal atom), employing hybrid functionals within the density functional theory. We analyze the electronic structure and the optical properties in terms of the absorption coefficients. By modeling the maximum device efficiency with respect to film thickness, we further discuss the optoelectronic response. The results help to understand fundamental physics of the Cu-based compounds in order to design and optimize very thin solar-energy devices.

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