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Facts and Artifacts in Optical and Structural Characterization of Emerging Materials for Renewable and Sustainable Energy

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The p-type emerging materials for photovoltaics such as inorganic chalcogenides and organohalide perovskites or other materials for renewable and sustainable energy applications in thin film or powder form are often reported with misleading/wrong optical and structural parameters. Thus, the credibility and significance of many published works should be questioned by the readers. Following a smart documentation by note taking including mind mapping, any should create an integrated protocol to find out the truth.

First issue concerns the XRD analysis. Several pathways will be given to identify correctly the crystalline phase, the lattice parameters, to find out and to prove the existence or absence of secondary phases and to determine the average crystallite sizes.

Second problem regards optical measurements and methods to extract the band gap. Can at least qualitatively observe the band gap difference within a samples batch? Is considered the possible differences between surfaces of the films and their bulk? Examples on inorganic chalcogenides and on organohalide perovskites will be given.

Also, tips and tricks concerning complementary techniques such as Raman spectroscopy and X-ray photoelectron spectroscopy will be revealed, needed to sustain the conclusions or, why not, to change even the initial scientific findings.

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