Redesigning Cs2Te: Workfunction Lowering and Quantum-Efficiency Preservation via Acetylation

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Abstract: Ultrabright photoinjector electron sources are a key technology for future light sources. The ability to tune the photocathode properties would allow us to optimize the source for a given set of requirements. For example, tuning the photoemission workfunction to lower photon energy while preserving the quantum efficiency (QE) allows a brighter electron beam for a given drive laser. Cs2Te is a well known high QE photoemissive material with a workfunction approximately 3 eV. It is desirable to lower its workfunction in order to become photoemissive due to visible photons while preserving its high QE. We show how such a modification can be designed using chemical intuition and electronic structure calculations. We predict [1] that the acetylation (reaction with acetylene gas) of Cs2Te will result in Cs2TeC2, a new member of a known class of ternary acetylides with synthesized members such as Cs2PdC2. Cs2TeC2 and all other ternary acetylides with the chemical formula of AMC2 or A2MC2 (A alkali, M transition metal or metalloid element, C2 acetylide) contain an infinite, rod-like 1D chain of [MC2] repeating unit, which is a 1D pi-electron system, embedded in an alkali matrix. By acetylating Cs2Te, we intuitively create a pi-electron system in it. Since pi-electron systems are typically coloured semiconductors with band gaps in the visible photon's range, it can be expected that the band-gap and potentially also the workfunction of Cs2Te gets reduced. Calculations indicate that the acetylation not only lowers the optical band gap, but also significantly lowers the workfunction of Cs2Te as well, down to 2.4 eV, while preserving its high QE. As opposed to Cs2Te, its acetylated version, Cs2TeC2, has highly anisotropic optical absorption and workfunction. Crystal surfaces running parallel with the rod-like substructures (based on [MC2] repeating units) exhibit the lowest workfunctions and are energetically most favorable. Other members of the ternary acetylide family of materials have similar photophysical properties. Details of the theoretical redesign of Cs2Te and photophysical properties of ternary acetylides will be presented.

[1] J.Z. Terdik, K. Nemeth, K.C. Harkay, J.H. Terry Jr., L. Spentzouris D. Velazquez, R. Rosenberg and G. Srajer, Phys. Rev. B, in press (2012).