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Computational Exploration of the Surface Properties of Cs2Te5 Photoemissive Material ANTHONY RUTH, Student, KAROLY NEMETH, Adjunct Professor of Physics, KATHERINE HARKAY, Physicist at Argonne, LINDA SPENTZOURIS, JEFF TERRY, Associate Professor of Physics — Cs2Te is a broadly used photoemissive material due to its exceptionally high quantum efficiency ($\sim 20\%$). Our group has recently predicted that the acetylation of this material (Cs2TeC2) would lower its workfunction down to about 2.4 eV from ~ 3 eV, and preserve its high quantum efficiency. Such a modification is advantageous because visible light can be used in the operation of such a photoemissive device instead of ultraviolet light. To explore other variants of Cs2Te, we conducted DFT-based computational analysis of the photoemissive properties of Cs2Te5 which is a known phase of Cs and Te. Cs2Te5 attracted our attention for its rod-like 1D Te substructures embedded in a Cs matrix. This structure is similar to Cs2TeC2 as Cs2TeC2 contains TeC2 polymeric rods in a Cs matrix. In addition to that, exploration of various Cesium Telluride phases is necessary to better understand the working of Cs2Te photocathodes. We have calculated surface energies, workfunctions, and optical absorption spectra of several different surfaces of Cs2Te5. A comparison of the properties of various Cs2Te5 surfaces and their utilization in photoemissive devices will be presented.

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