Searching for low-workfunction phases in the Cs-Te system: The case of Cs_2Te_5

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We have computationally explored workfunction values of Cs_2Te_5 surfaces, an existing crystalline phase of the Cs-Te system and a small bandgap semiconductor, in order to search for reduced workfunction alternatives of Cs_2Te that preserve the exceptionally high quantum efficiency of the Cs_2Te seasoned photoemissive material. We have found that the Cs_2Te_5(010) surface exhibits a workfunction value of ≈1.9 eV when it is covered by Cs atoms. Cs_2Te_5 is analogous to our recently proposed low-workfunction materials, Cs_2TeC_2, and other ternary acetylides [J. Z. Terdik *et al.*, Phys. Rev. B **86**, 035142 (2012)], in as much as it also contains quasi one-dimensional substructures embedded in a Cs-matrix, forming the foundation for anomalous workfunction anisotropy and low workfunction values. The one-dimensional substructures in Cs_2Te_5 are polytelluride ions in a tetragonal rod-like packing. Cs_2Te_5 has the advantage of simpler composition and availability as compared to Cs_2TeC_2; however, its low workfunction surface is less energetically favored to the other surfaces than in Cs_2TeC_2. A significant and remarkable advantage of Cs_2Te_5 as compared to Cs_2Te is its high optical absorption of visible photons that can allow for high quantum efficiency electron emission at visible photon energies. © *2013 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4804155]

I. INTRODUCTION

Cesium telluride (Cs_2Te) has been known since the 1950s as an exceptionally high quantum efficiency photoemissive material;[1] it can turn as much as ≈20% of the incident ultraviolet photons into emitted electrons.[2] Cesium telluride also has the advantage of relatively long operational lifetime, 20–30 times longer than that of competing multi-alkali antimonide photocathodes, such as K_2CsSb and (Cs)Na_3KSb. While K_2CsSb and (Cs)Na_3KSb require ultra-high vacuum for operation, Cs_2Te can operate in orders of magnitudes lower levels of vacuum.[3] In order to further enhance the photoemissive properties of Cs_2Te for certain applications, modifications are required that decrease its workfunction from the ≈3.0 eV down to the visible light spectrum (1.5–3.0 eV) while preserving its high quantum efficiency. Such modifications can lead to, for example, for high brightness electron guns,[3,4] better pulse shaping of the incident photons in the visible spectrum and eliminating the need for wavelength down-conversion. Wavelength down-conversion is used to convert the typically near-infrared photons of the laser source to ultraviolet wavelength which causes a great loss of the intensity of the initial laser-beam. One possible way to an improved photoemissive material that we recently proposed[5] is the acetylation of Cs_2Te leading to Cs_2TeC_2, a new member of the existing family of ternary acetylide[6–8] compounds. Electronic structure calculations predict that the new Cs_2TeC_2 and other existing ternary acetylides, such as Cs_2PdC_2, would have similarly high quantum efficiencies as Cs_2Te but significantly lower 2.0–2.4 eV workfunctions.

An alternative route to the acetylation in developing improved photoemissive analogues/derivatives of Cs_2Te might be in the exploration of photoemissive properties of other Cs-Te phases. A comprehensive review of alkali tellurides by Smith and Ibers[9] called our attention to Cs_2Te_5, an existing[10] crystalline phase of Cs and Te. Remarkably, the Te_5^{2-} polytelluride anions in Cs_2Te_5 self organize to ≈4 Å wide wavy ribbons of Te with continuous covalent Te-Te networks, which are embedded into a Cs matrix, such as shown in Fig. 1. In the wavy Te-ribbons, six-membered rings of Te in chair-conformation are connected via common vortices into quasi 1D chains, as depicted in Fig. 2. These quasi 1D substructures of Cs_2Te_5 resemble the rod-like polymeric $[-Te-C\equiv C-]_n^{2n-}$ substructures that are responsible for the improved photoemissive properties of Cs_2TeC_2. This structural analogy directed our attention towards the computational analysis of Cs_2Te_5 to check whether it can potentially serve as an improvement to Cs_2Te and ternary acetylides.

II. METHODOLOGY

The electronic structure calculations in the present study have been carried out using the Quantum Espresso program package.[11] The Perdue-Burke-Ernzerhof (PBE) exchange-correlation potential[12] has been used with norm-conserving Cs and Te pseudopotentials identical to those in our study for Cs_2TeC_2 in Ref. 5. The wavefunction-cutoff was 80 Ry. The k-space grids were at least $6\times6\times6$ large for optimizations, the residual forces on fractional coordinates were less than 4×10^{-4} Ry/au, and residual pressure on the unit cell

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