

Abstract Submitted  
for the TSF21 Meeting of  
The American Physical Society

**Stability and Optical Properties of Copper-Cysteamine with Halogens by First Principles Calculations**<sup>1</sup> NOURA ALKHALDI, MUHAMMAD N. HUDA, University of Texas at Arlington — Copper cysteamine (Cu-Cy) is known as a photosensitizer that can be activated by visible light, X-rays, microwaves, and ultrasound to generate reactive oxygen species (ROS). ROS which are produced by Cu-Cy can be used to treat the cancer, infection diseases as well to decontaminate the water from the microbes, and organic dye molecules. Hence, it is important to understand the electronic and optical properties of Cu-Cy material. In this presentation, we will show results from our density functional theory (DFT) calculations of the stability of Cu-Cy structures as well the electronic and optical properties of Cu-Cy-X (X= F, Cl, Br, I). Different spin-multiplicities as well spin-orbit-coupling (SOC) are considered to understand the electron transition from the occupied to the unoccupied bands. Defects such as Cu-vacancy and X-vacancy are made in the pristine structures of Cu-Cy-X to see how those affect the stability of the structures. Reaction barriers of Cu atom in Cu-Cy-X are calculated to mimic the Cu leaching which are observed experimentally. Our theoretical results show good agreements with the experimental data.

<sup>1</sup>NDA acknowledges the support of the Saudi Arabian Cultural Mission and University of Hafr Albatin. MNH was supported by the National Science Foundation (NSF) award 1609811. NDA and MNH gratefully acknowledge the generous computations time awarded by the Texas Advanced Computing Center (TACC).

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Date submitted: 24 Sep 2021

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