First-principles study electronic and optical properties of silver chloride photocatalyst
Abdulmutta Thatribu1*, Teparsrksorn Pengpan2
1Physics major, Department of Science, Faculty of Science and Technology, Prince of Songkla University, Pattani Campus, Pattani 94000, Thailand
2Department of Physics, Faculty of Science, Prince of Songkla University, Hat Yai Campus, Hat Yai, Songkla 90110, Thailand
*E-mail: abdulmutta.t@psu.ac.th

Abstract: In this work we study the electronic and optical properties of the photocatalytic materials AgCl. Based on Density Functional Theory (DFT) with Generalized Gradient Approximation (GGA), optimized lattice parameter, band gap, density of states, and dielectric functions of the bulk AgCl are calculated. To accurately determine the AgCl band gap, its band energies are corrected by using the GW and QPscGW method. Further to the DFT-GGA and GW electronic band structure calculations of the bulk AgCl, the dielectric functions, which manifest the optical properties, are calculated by random phase approximation (RPA) and Bethe-Salpeter equation (BSE), that includes the electron-hole correlation effect and show strong excitonic peaks. Then, we compare our theoretical results with the available experimental data and finally discuss the key issues that influence the photocatalytic properties.

Keywords: Density functional theory; Electronic structure; Bethe-Salpeter equation; Photocatalytic